

Supplementary Materials

for the paper

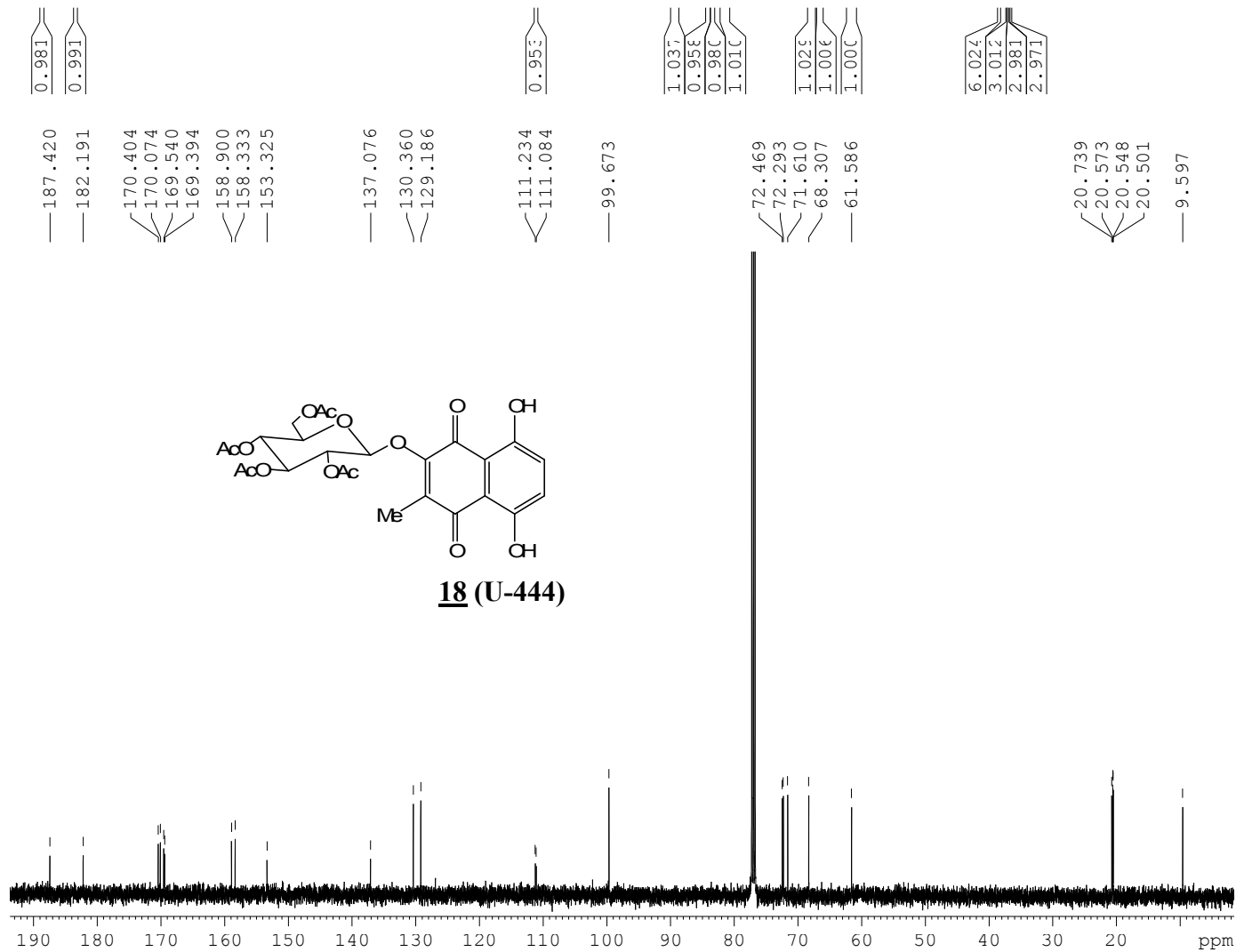
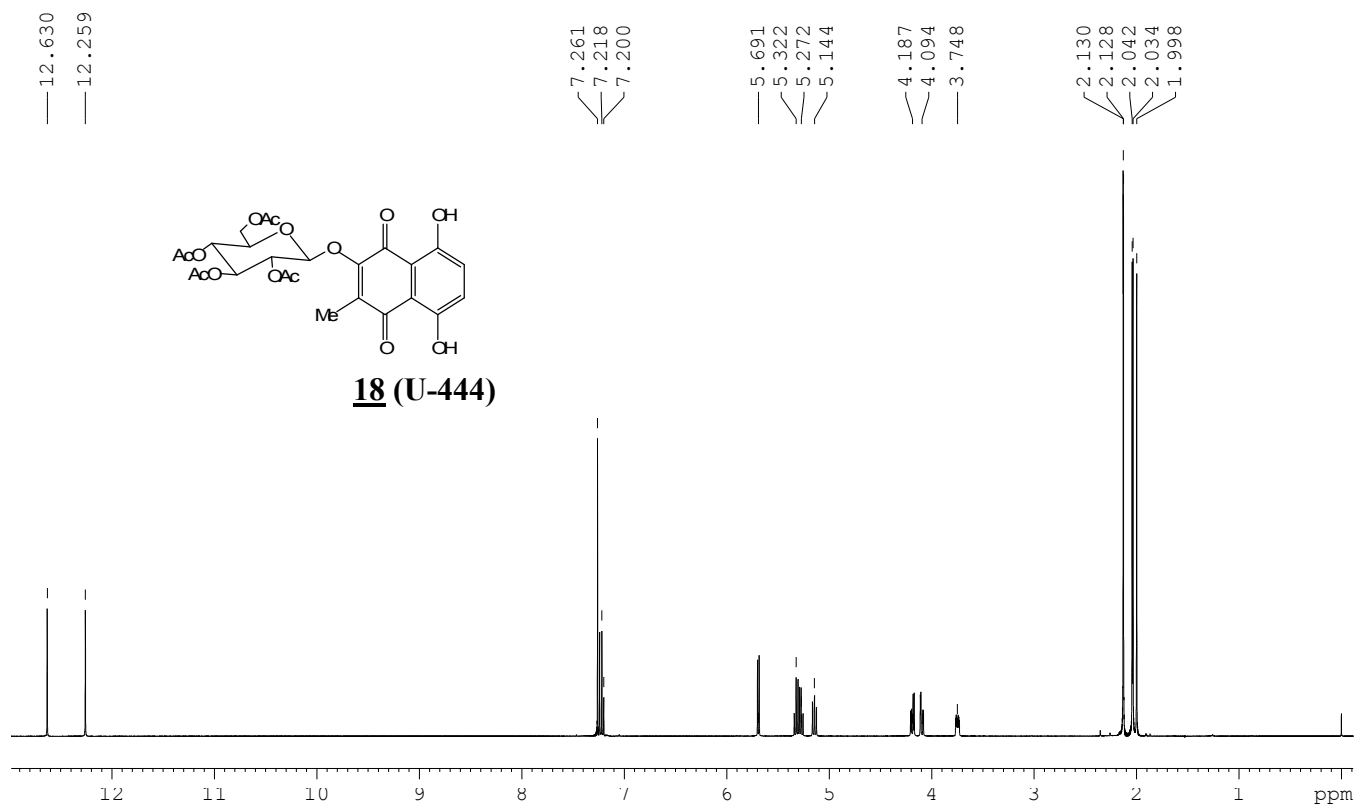
“Synthesis, Cytotoxic Activity Evaluation and Quantitative Structure-Activity Analysis of Substituted 5,8-Dihydroxy-1,4-Naphthoquinones and their O- and S-Glycoside Derivatives Tested Against Neuro-2a Cancer Cells”

Sergey Polonik, Galina Likhatskaya, Yuri Sabutski, Dmitry Pelageev, Vladimir Denisenko, Evgeny Pisyagin, Ekaterina Chingizova, Ekaterina Menchinskaya, Dmitry Aminin.

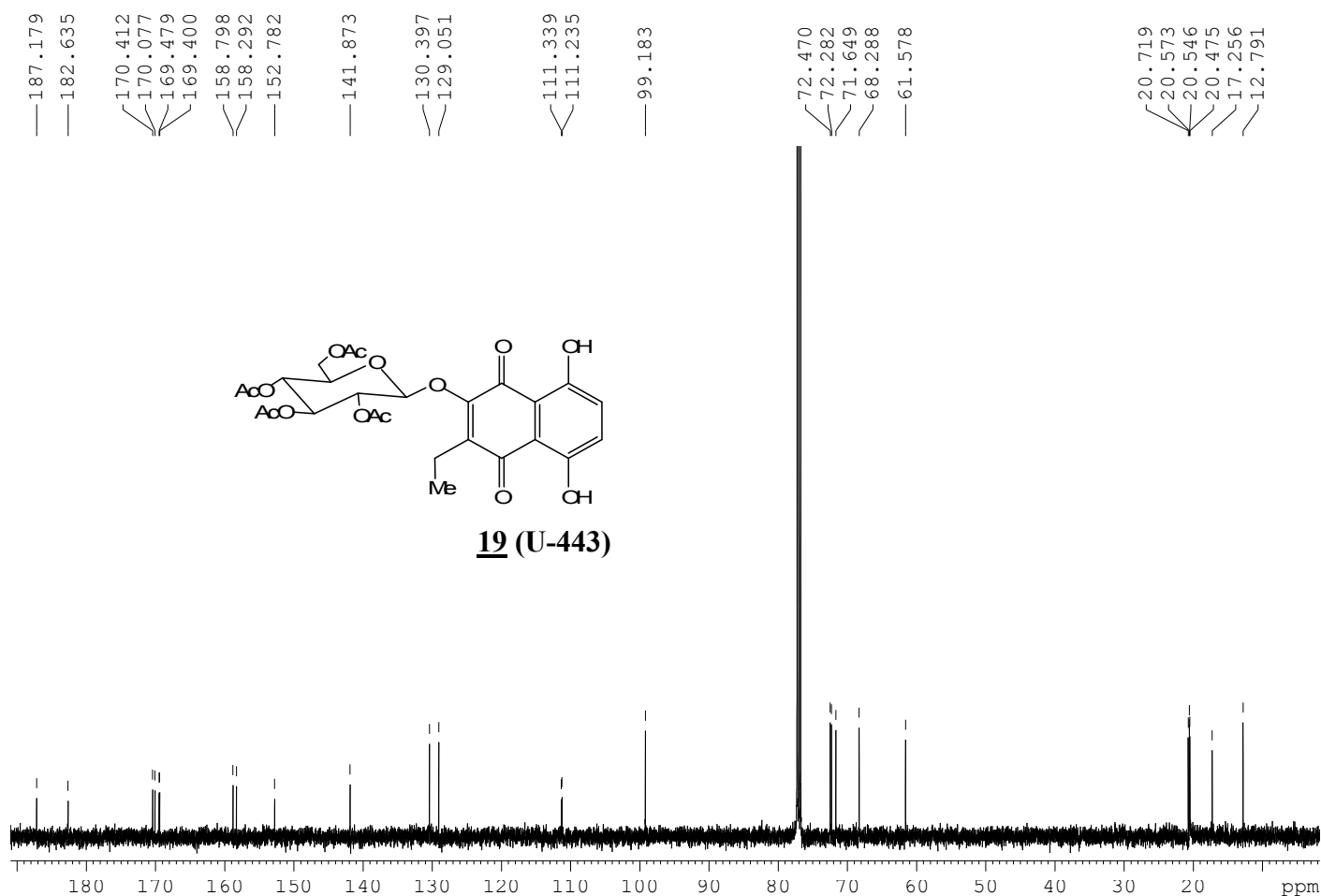
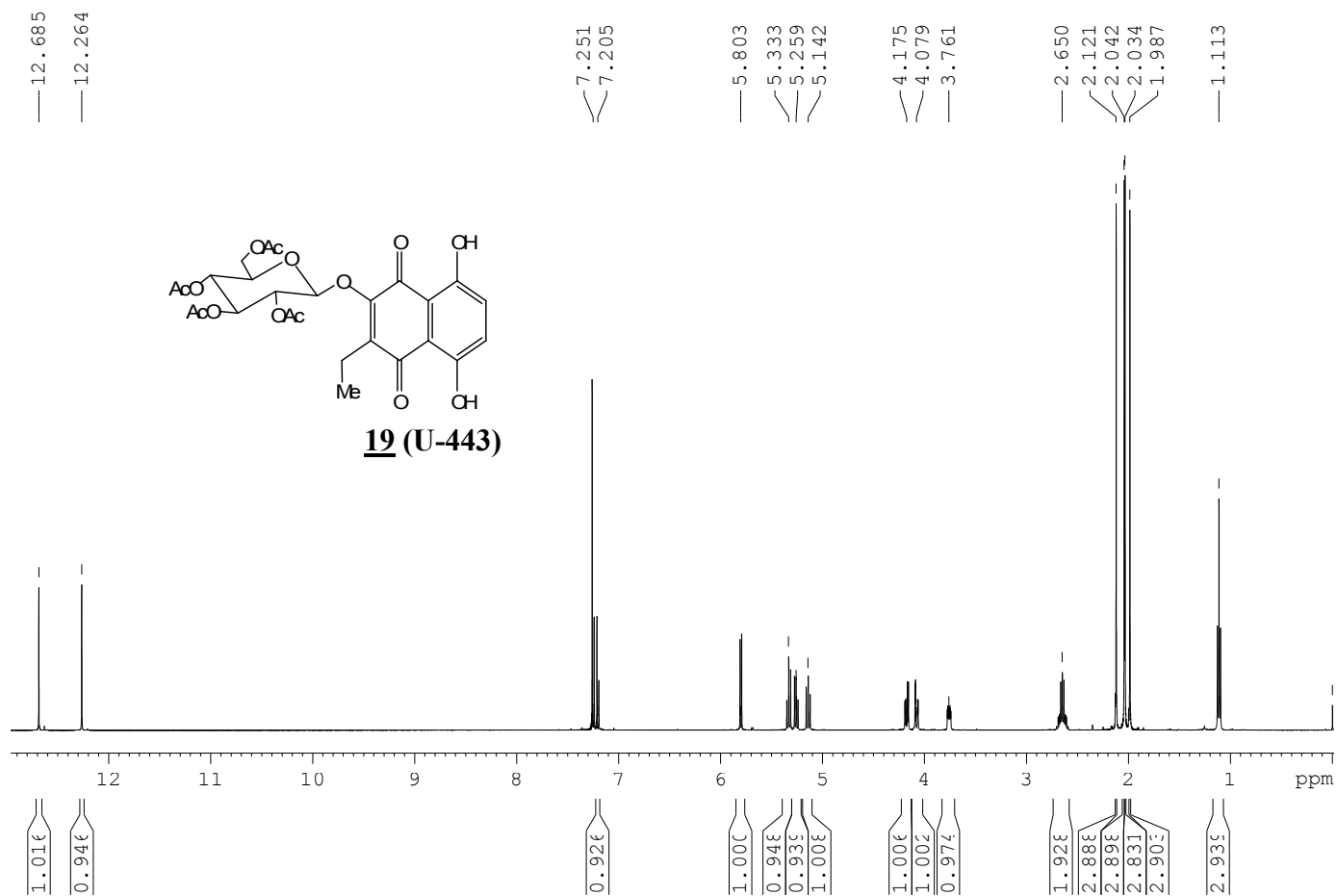
Content

¹H and ¹³C NMR spectra for synthesized compounds S2-S34

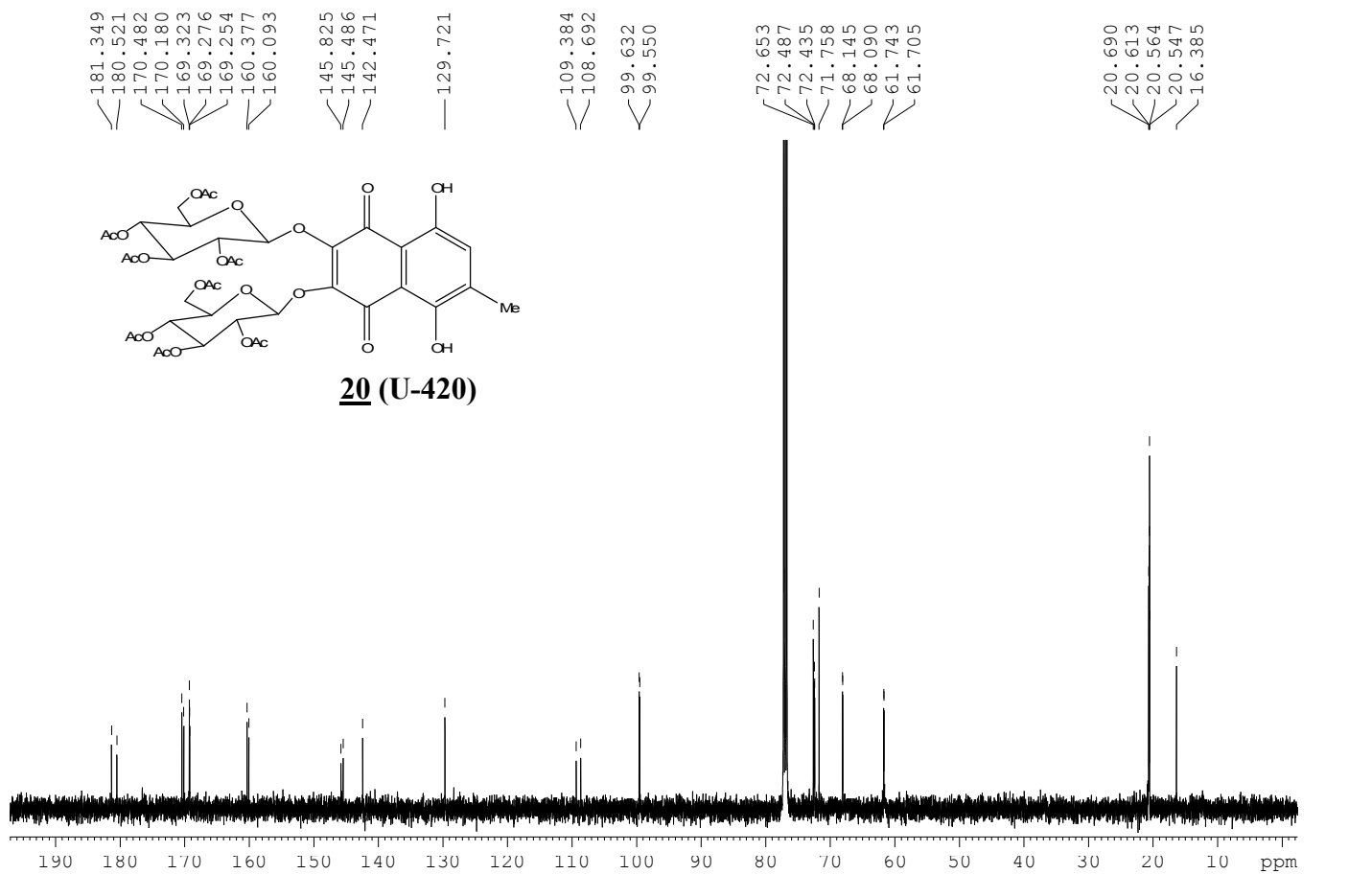
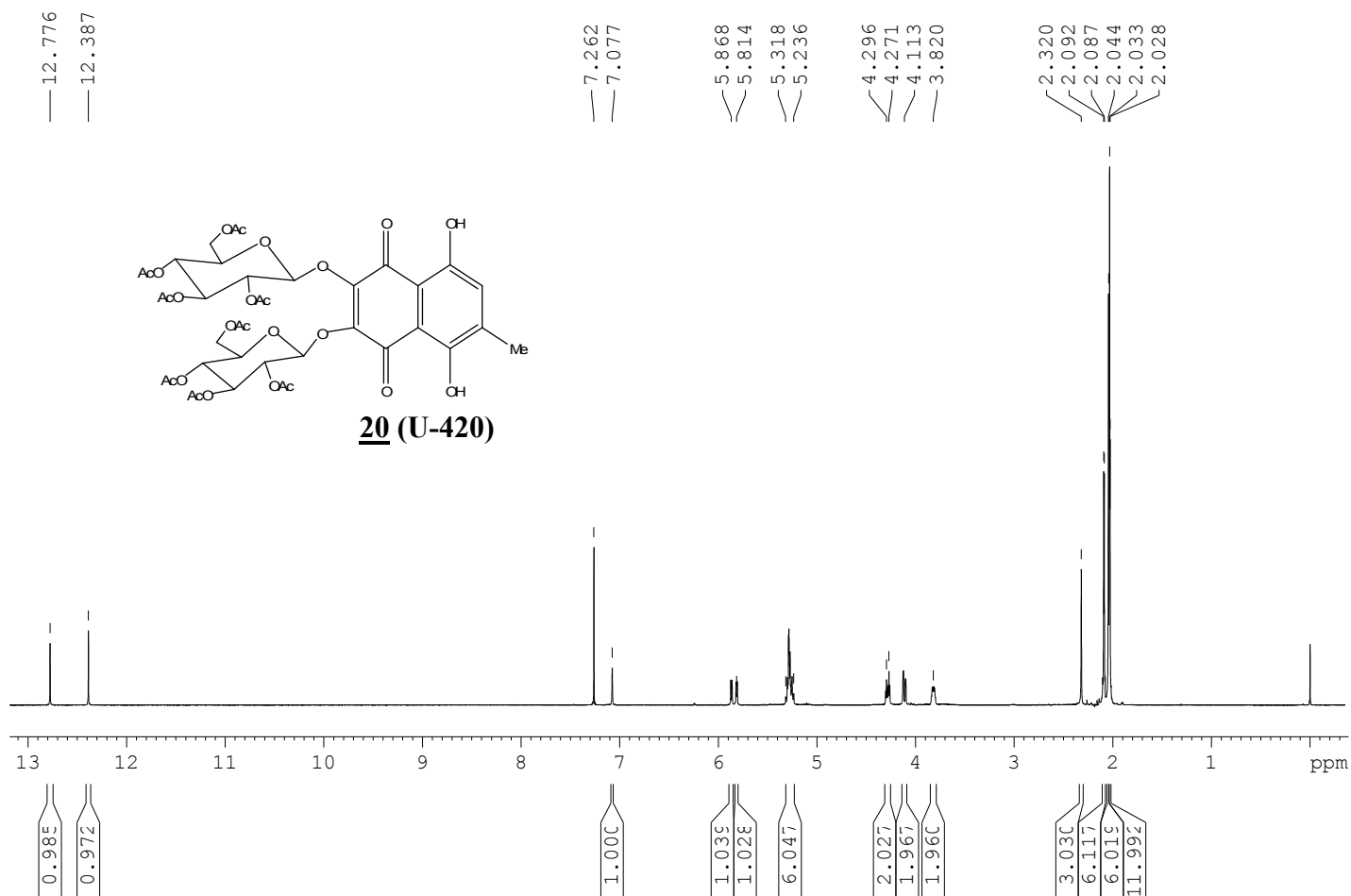
2-(Tetra-O-acetyl- β -D-glucopyranosyl-1-oxy)-5,8-dihydroxy-3-methylnaphthalene-1,4-dione **18** (U-444), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



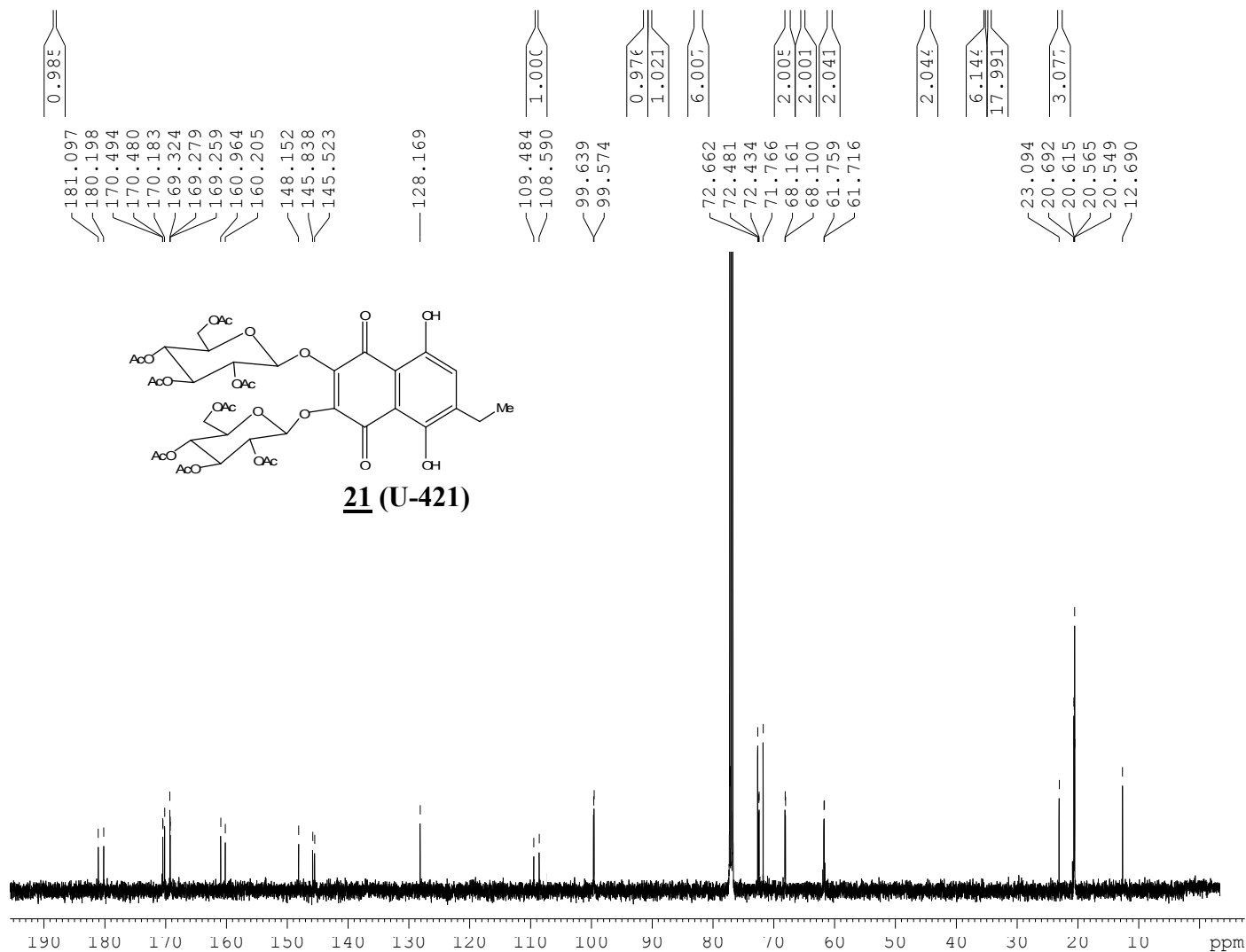
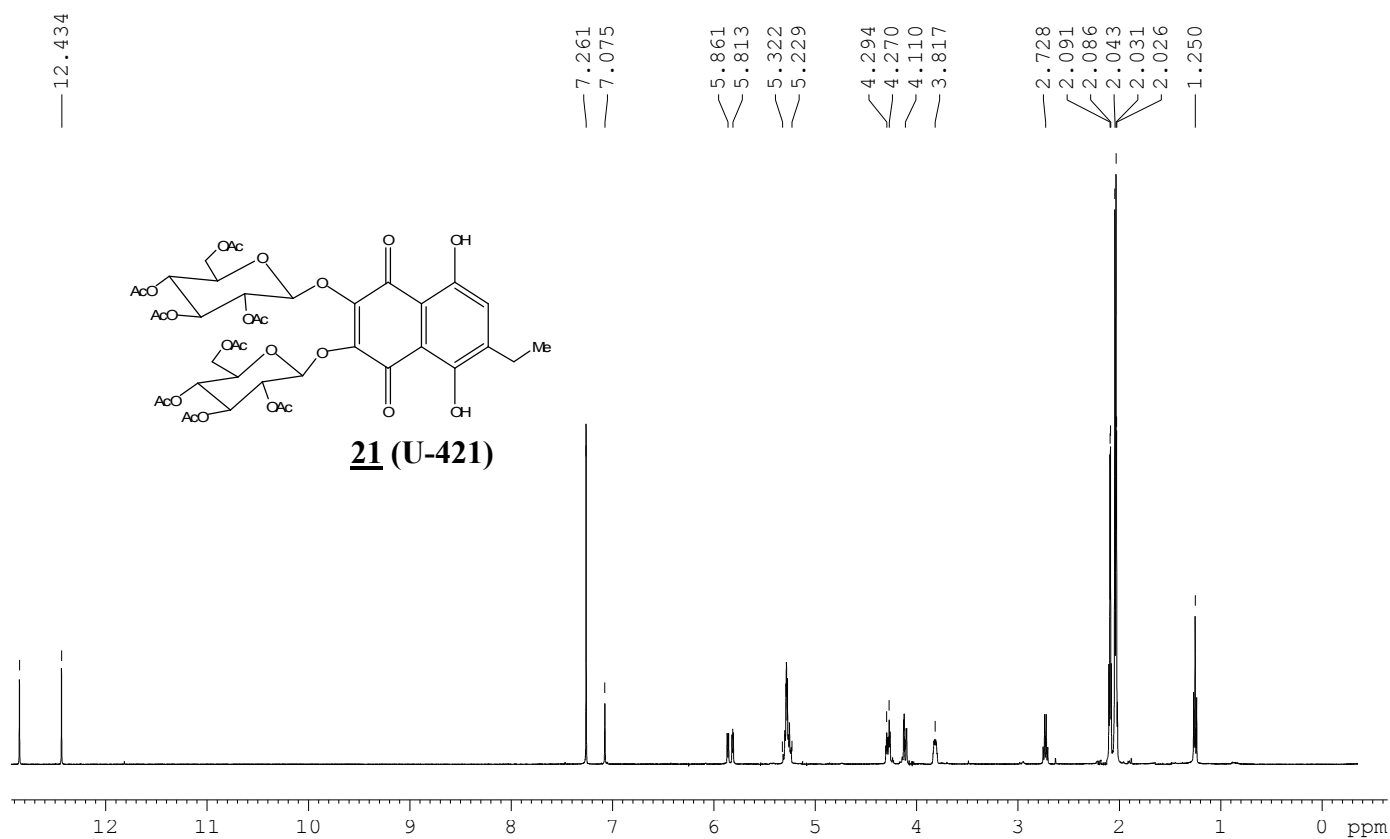
2-(Tetra-O-acetyl- β -D-glucopyranosyl-1-oxy)-3-ethyl-5,8-dihydroxynaphthalene-1,4-dione **19** (U-443), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



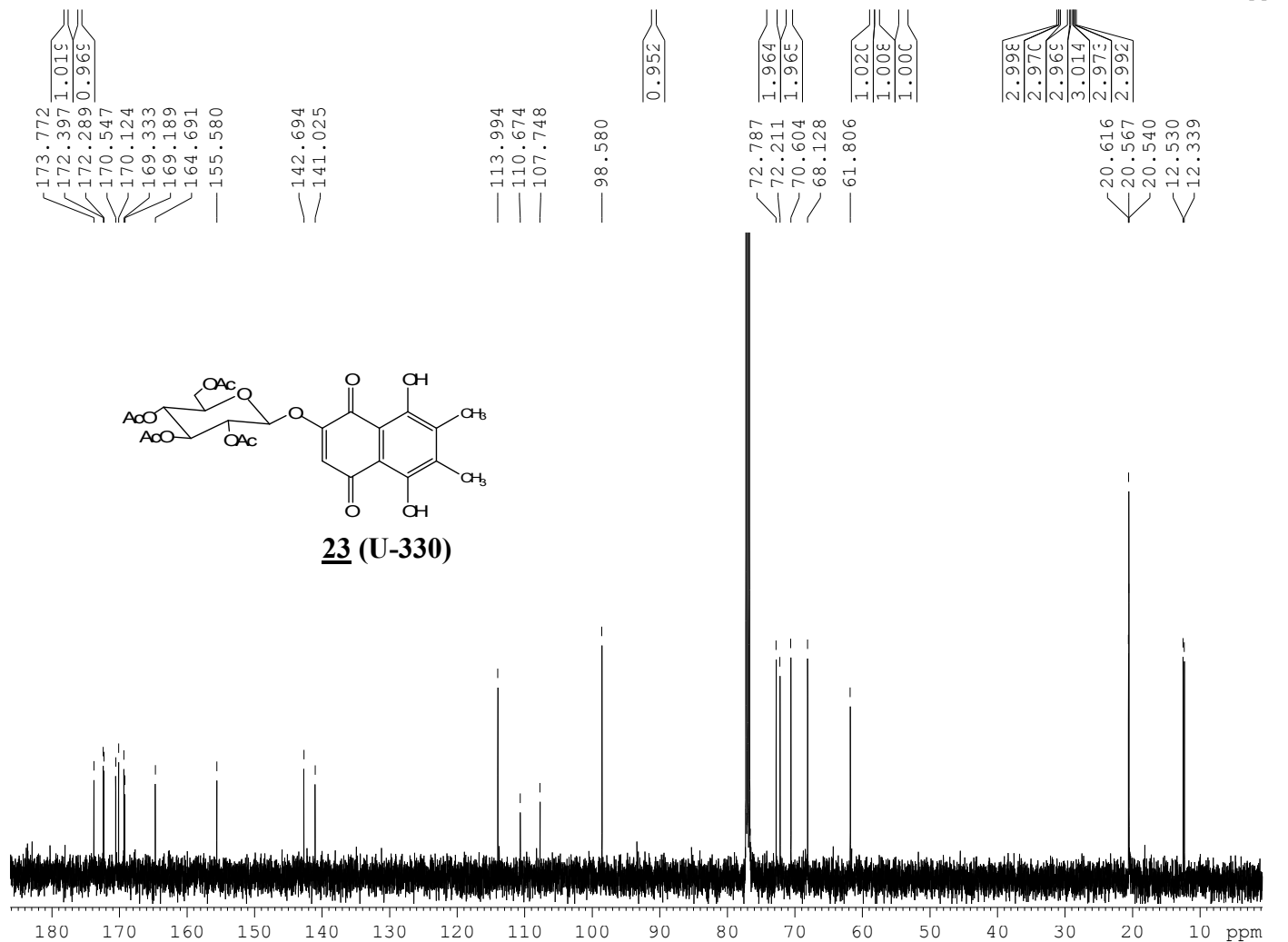
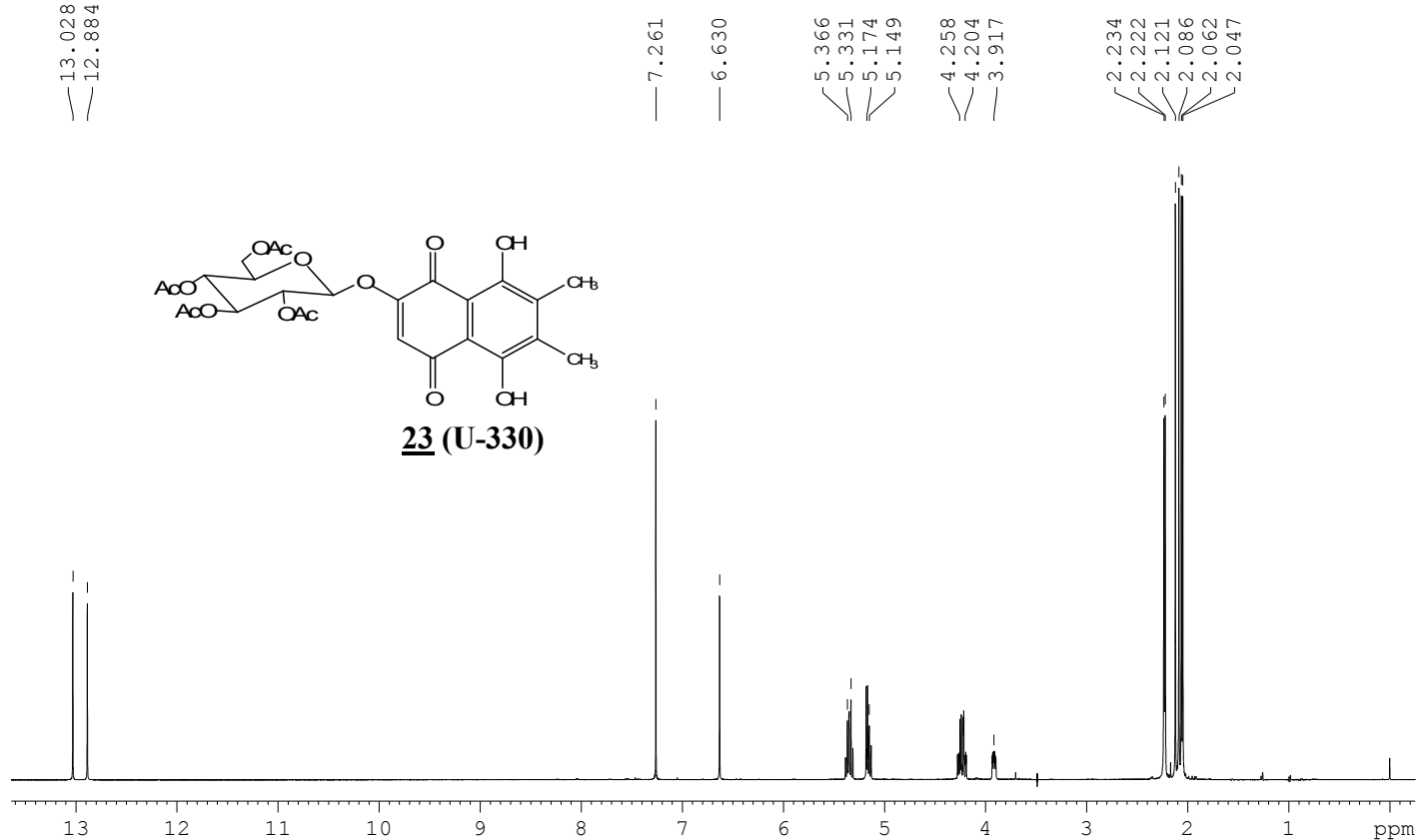
2,3-Bis(tetra-O-acetyl- β -D-glucopyranosyl-1-oxy)-5,8-dihydroxy-6-methylnaphthalene-1,4-dione **20** (U-420), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



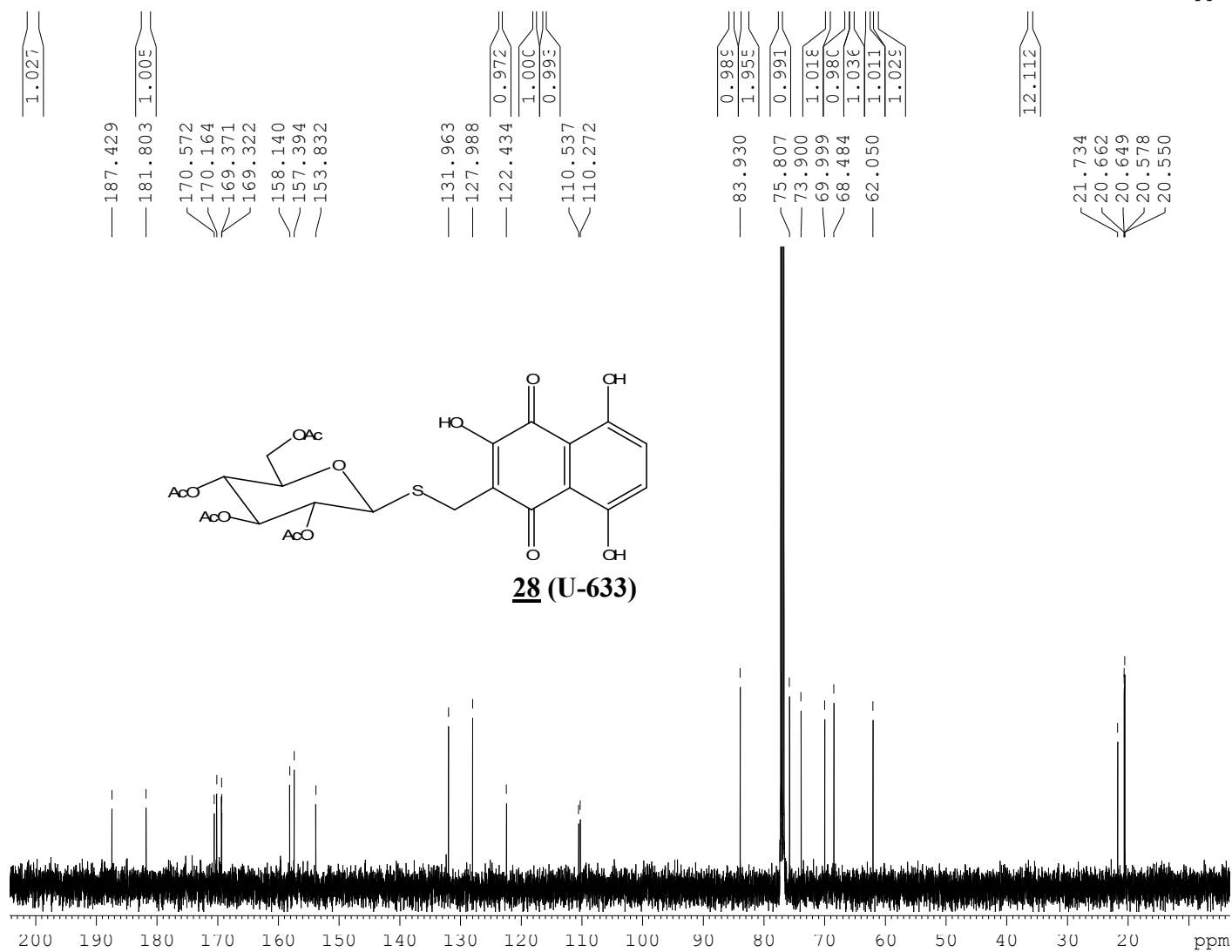
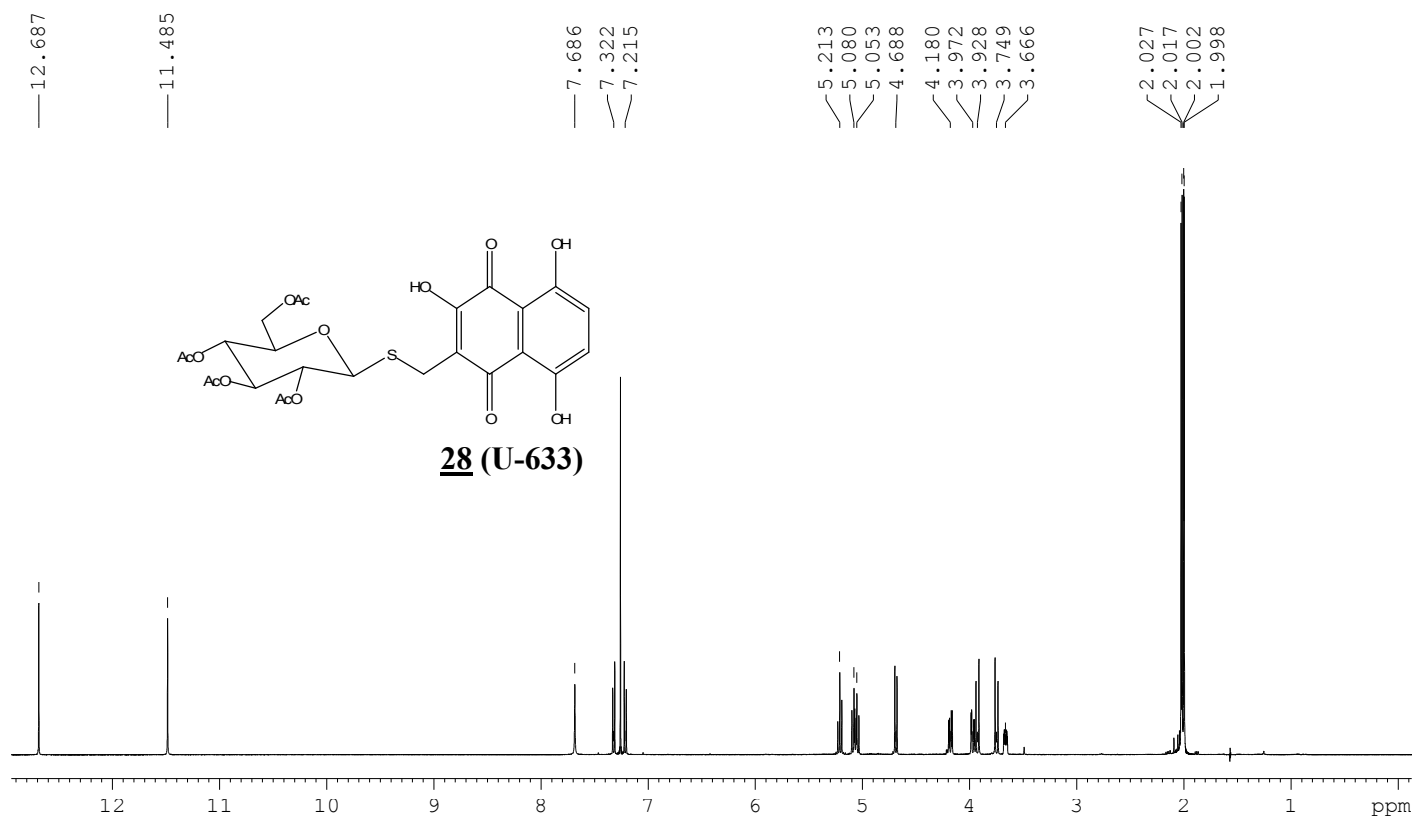
2,3-Bis(tetra-O-acetyl- β -D-glucopyranosyl-1-oxy)-6-ethyl-5,8-dihydroxynaphthalene-1,4-dione **21** (U-421), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



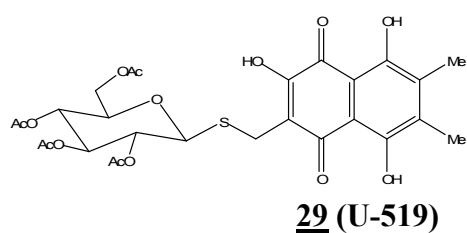
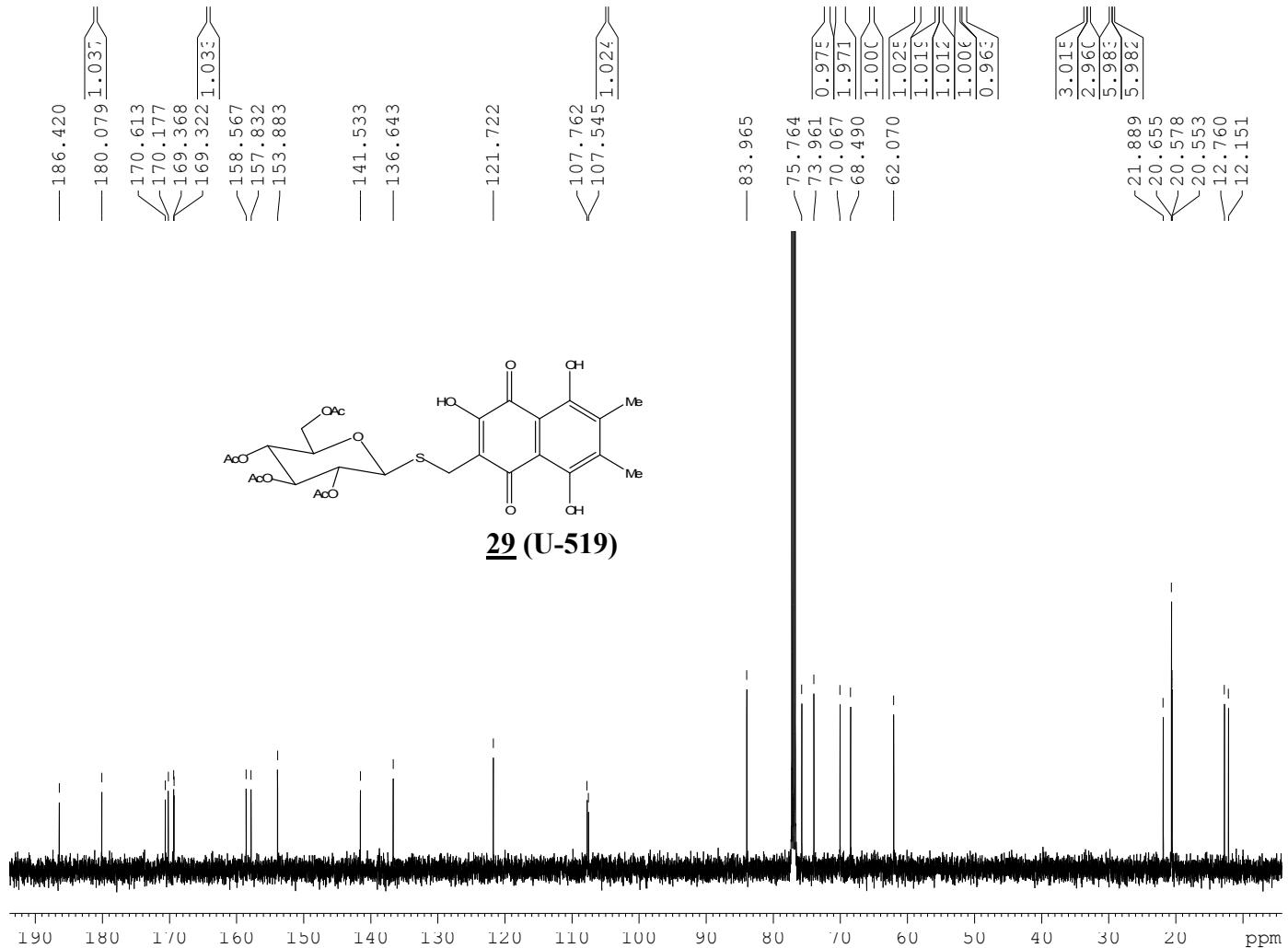
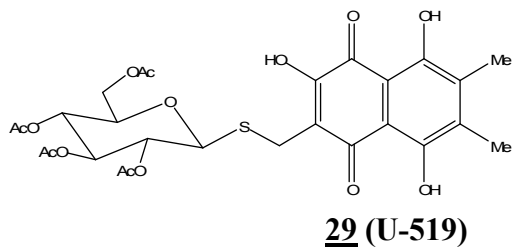
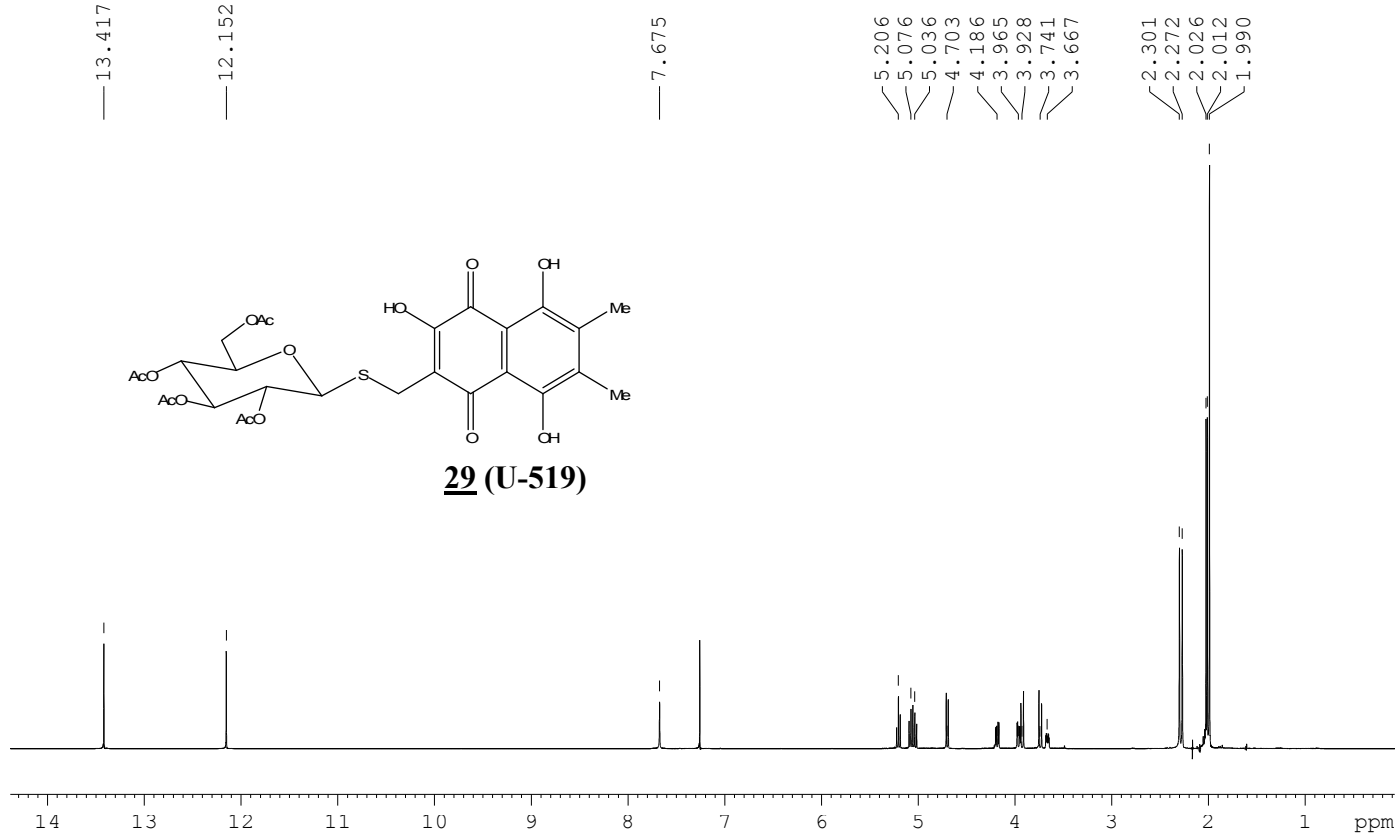
2-(Tetra-O-acetyl- β -D-glucopyranosyl-1-oxy)-5,8-dihydroxy-6,7-dimethylnaphthalene-1,4-dione **23** (U-330), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



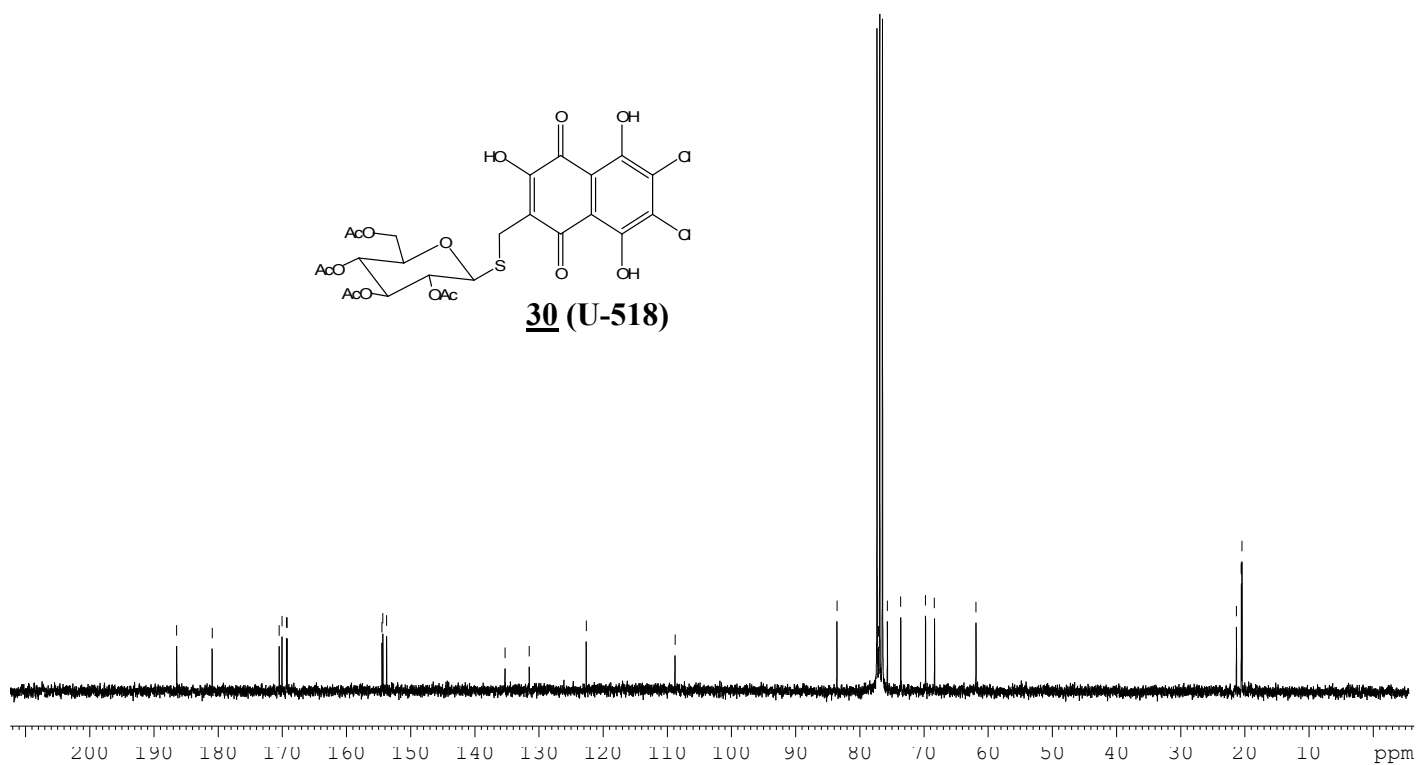
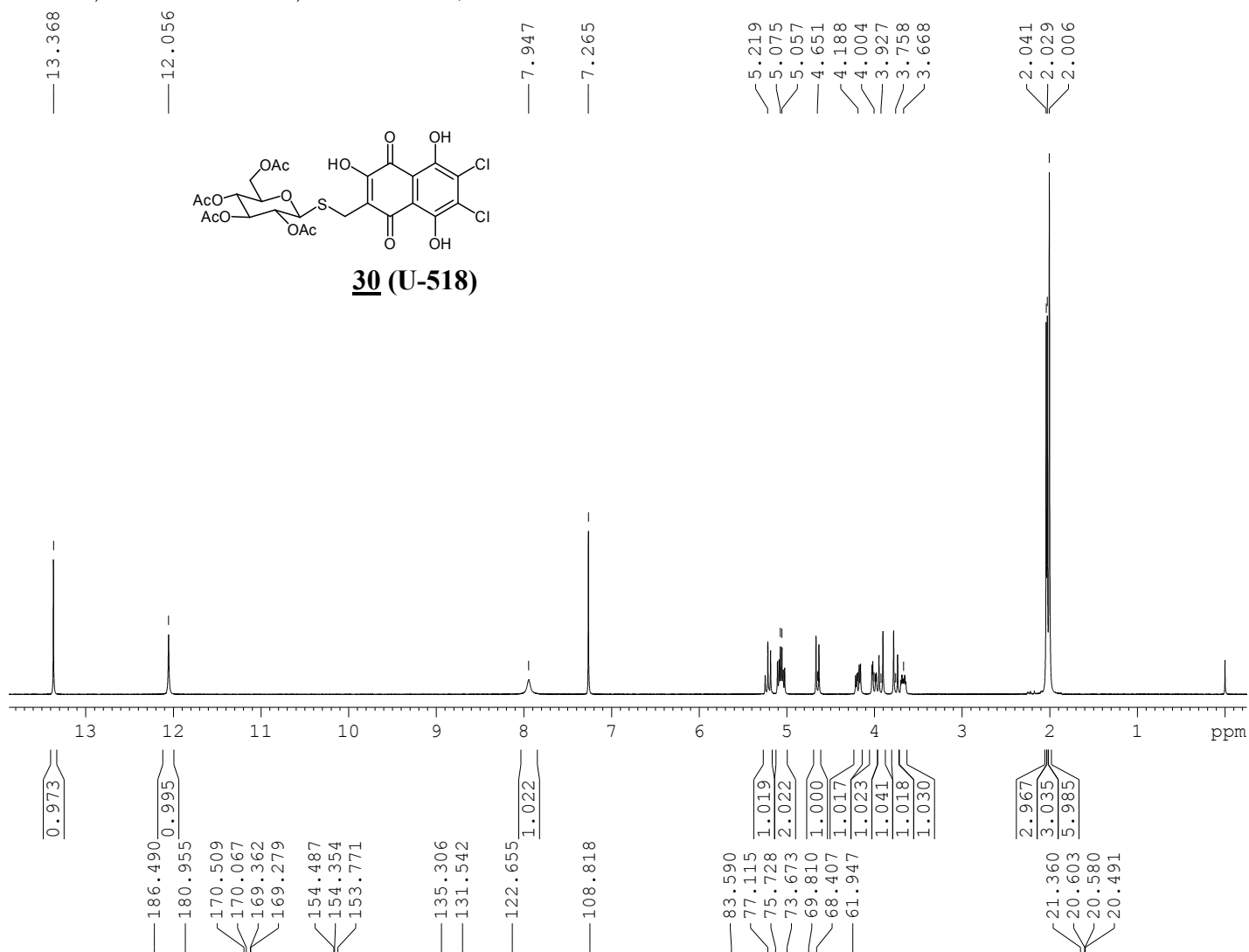
3-(Tetra-O-acetyl- β -D-glucopyranosyl-1-thiomethyl)-2,5,8-trihydroxynaphthalene-1,4-dione **28** (U-633), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



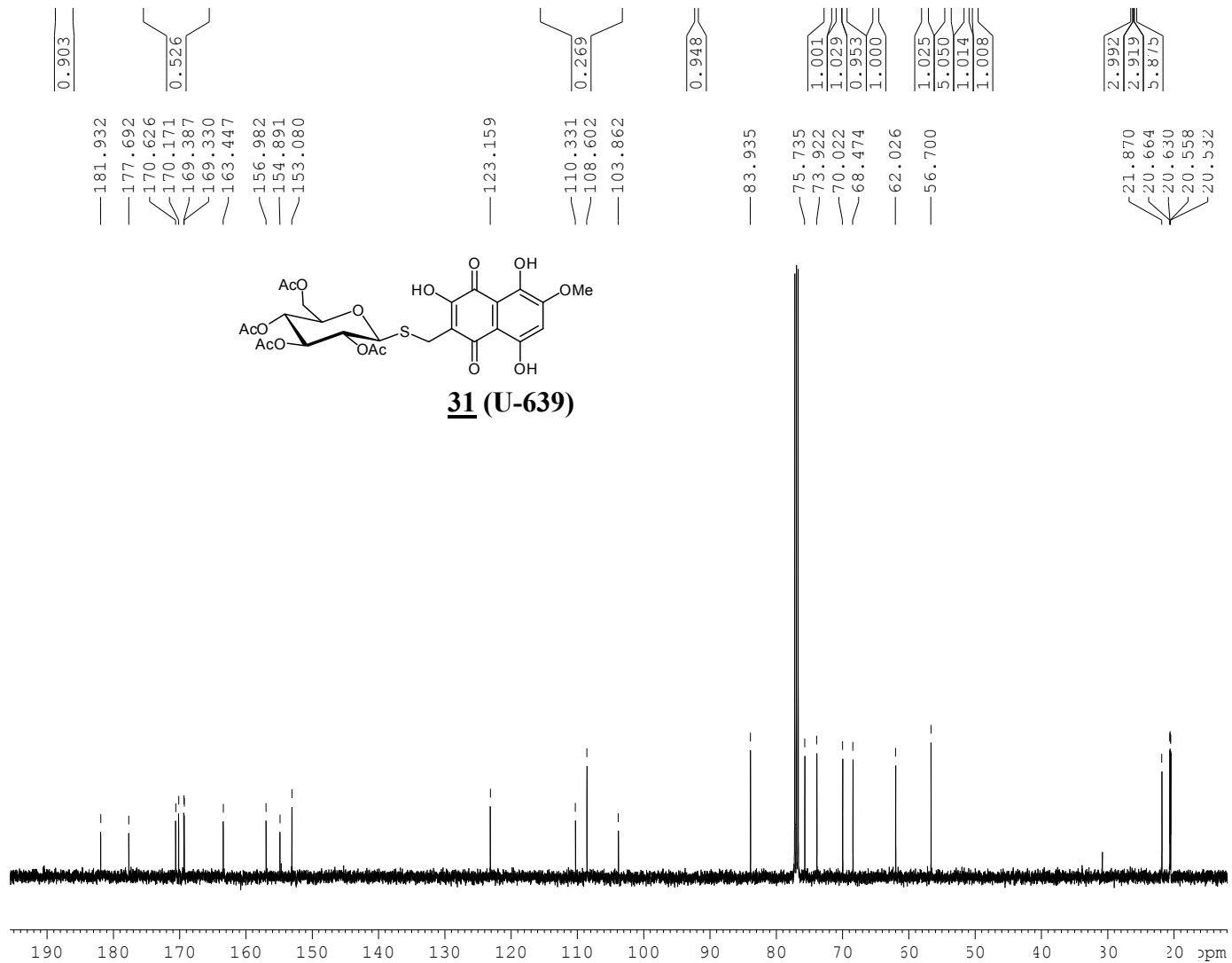
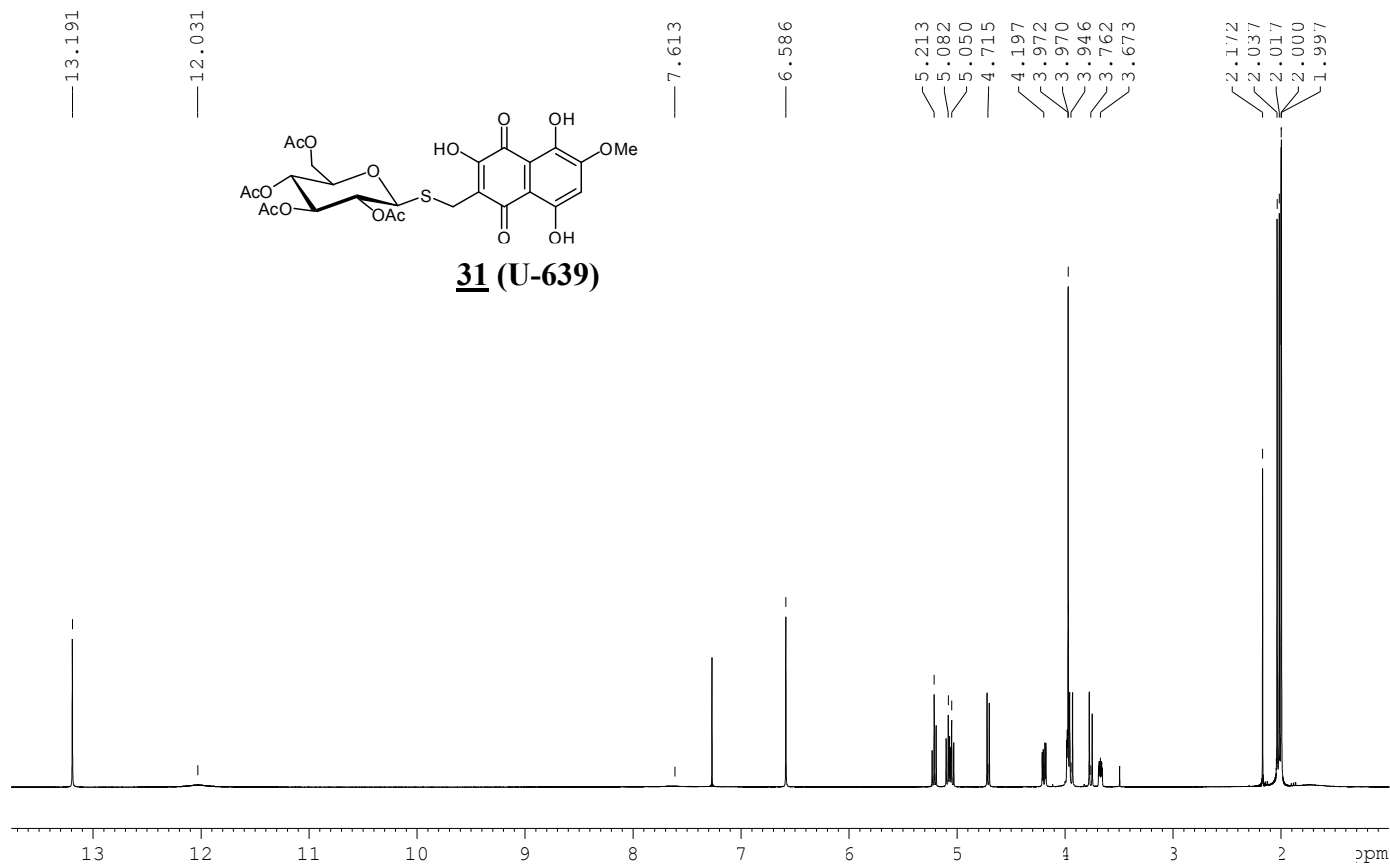
3-(Tetra-O-acetyl- β -D-glucopyranosyl-1-thiomethyl)-2,5,8-trihydroxy-6,7-dimethylnaphthalene-1,4-dione **29** (U-519), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



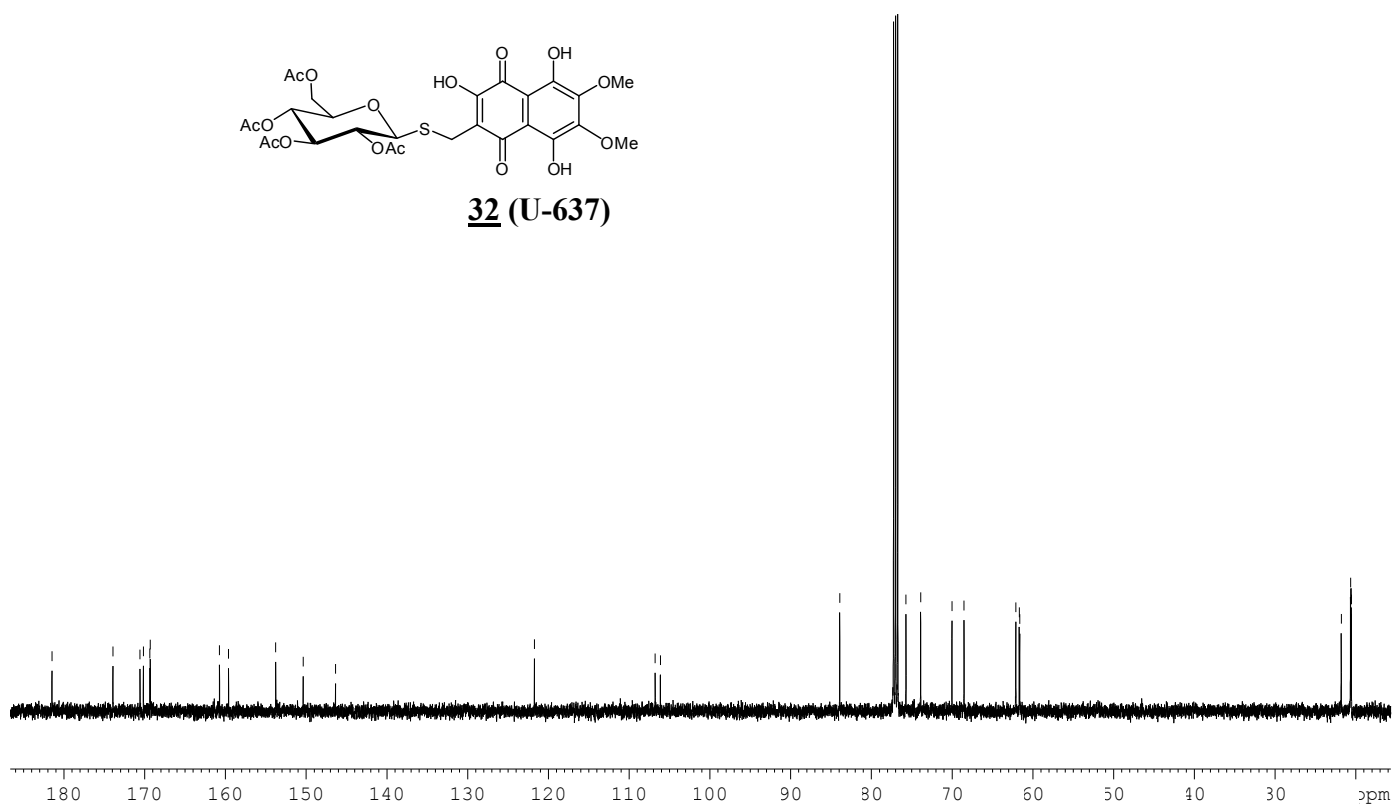
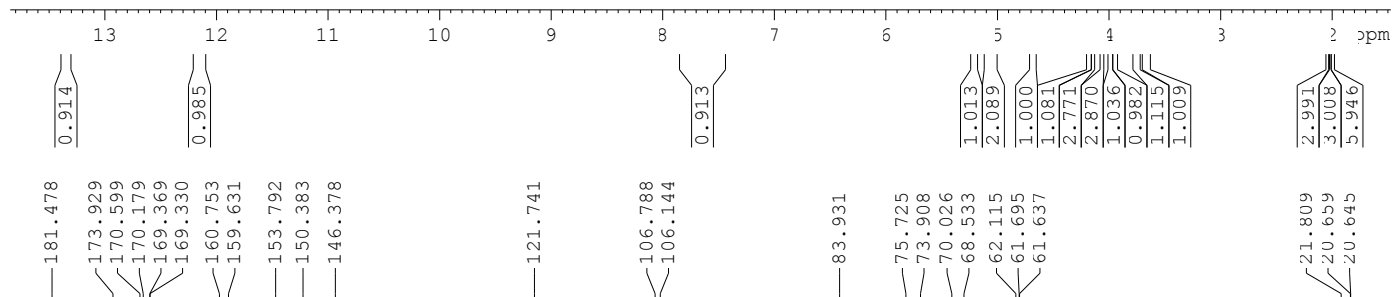
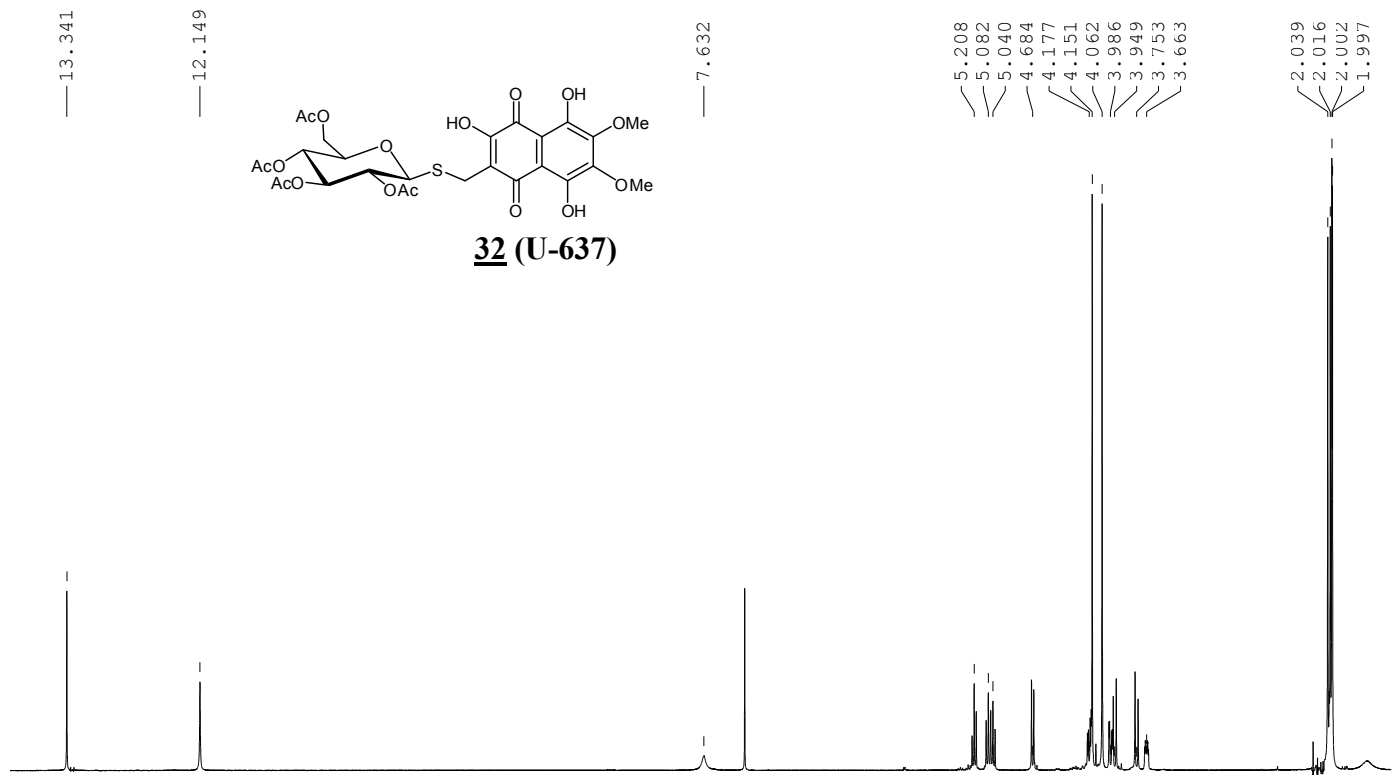
3-(Tetra-O-acetyl- β -D-glucopyranosyl-1-thiomethyl)-6,7-dichloro-2,5,8-trihydroxynaphthalene-1,4-dione **30** (U-518), (^1H NMR - 300 MHz, ^{13}C NMR - 75 MHz, solvent - CDCl_3)



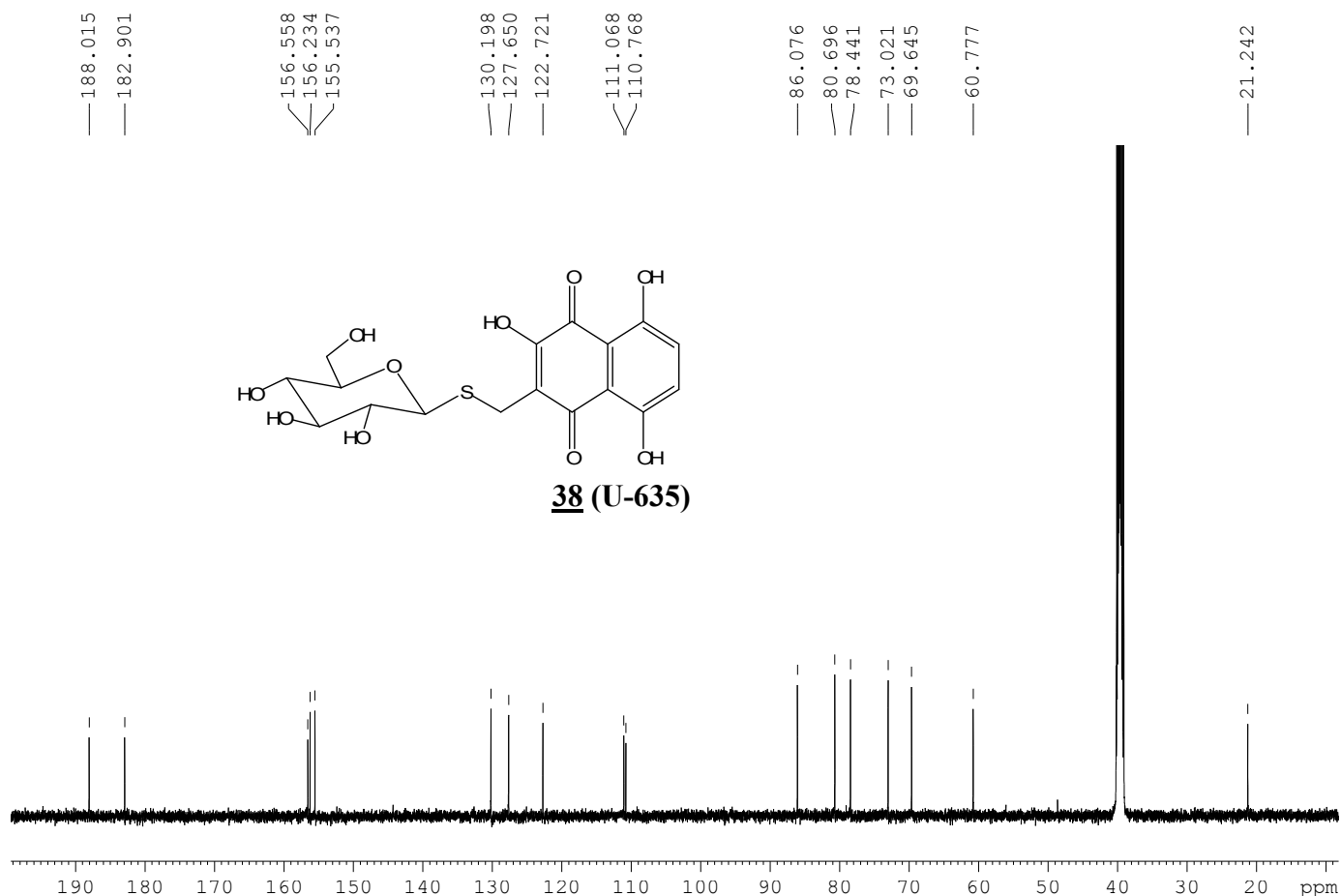
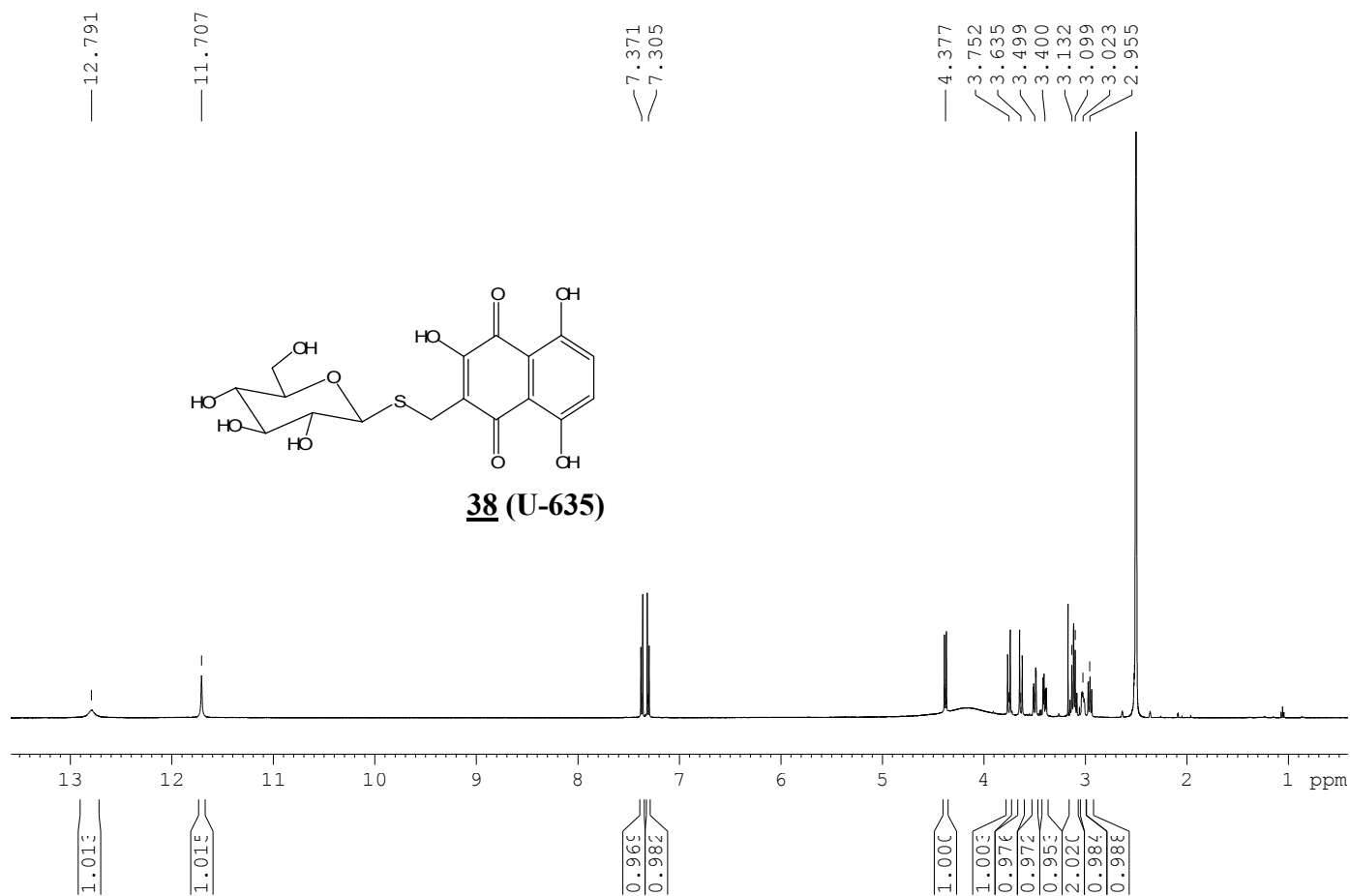
3-(Tetra-O-acetyl- β -D-glucopyranosyl-1-thiomethyl)-2,5,8-trihydroxy-7-methoxynaphthalene-1,4-dione **31** (U-639), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



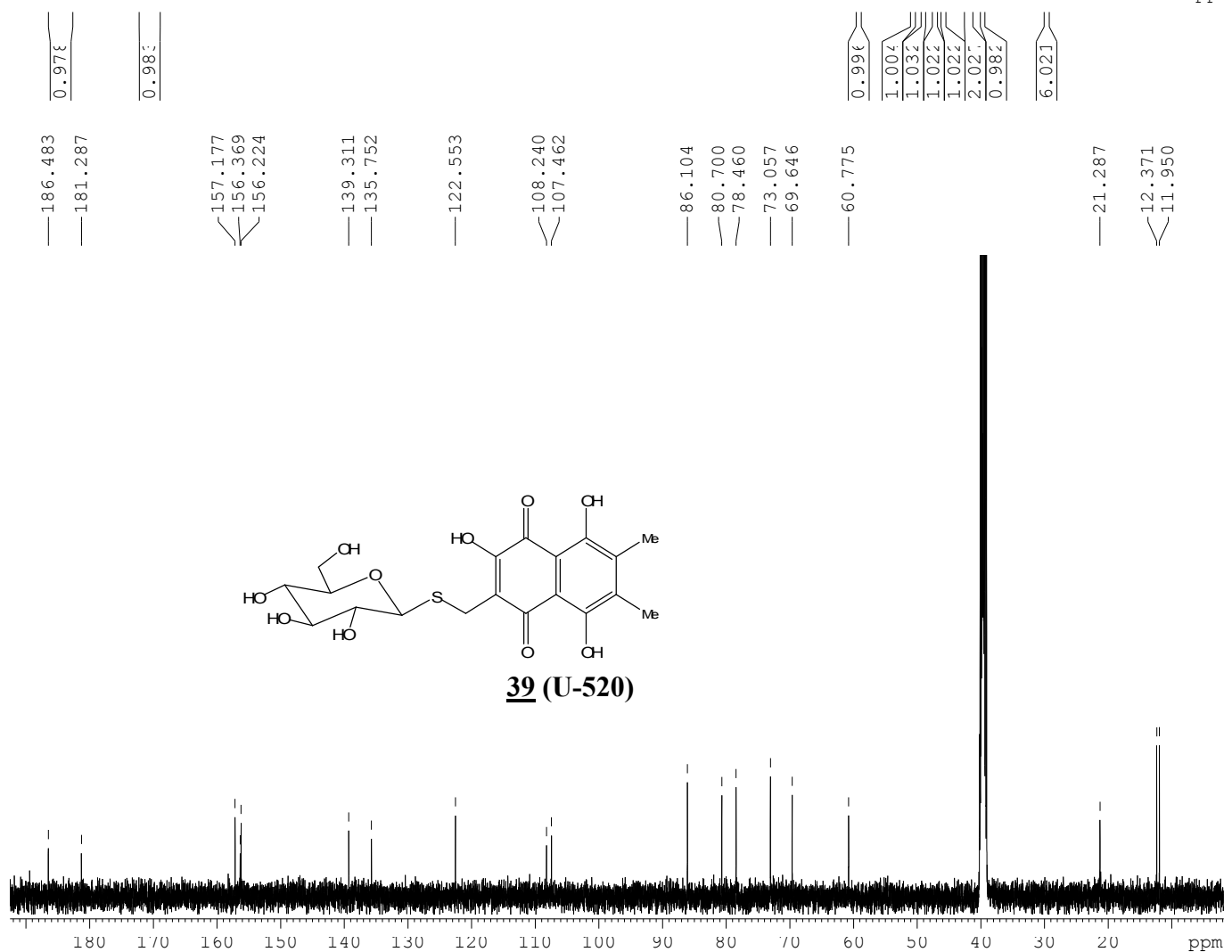
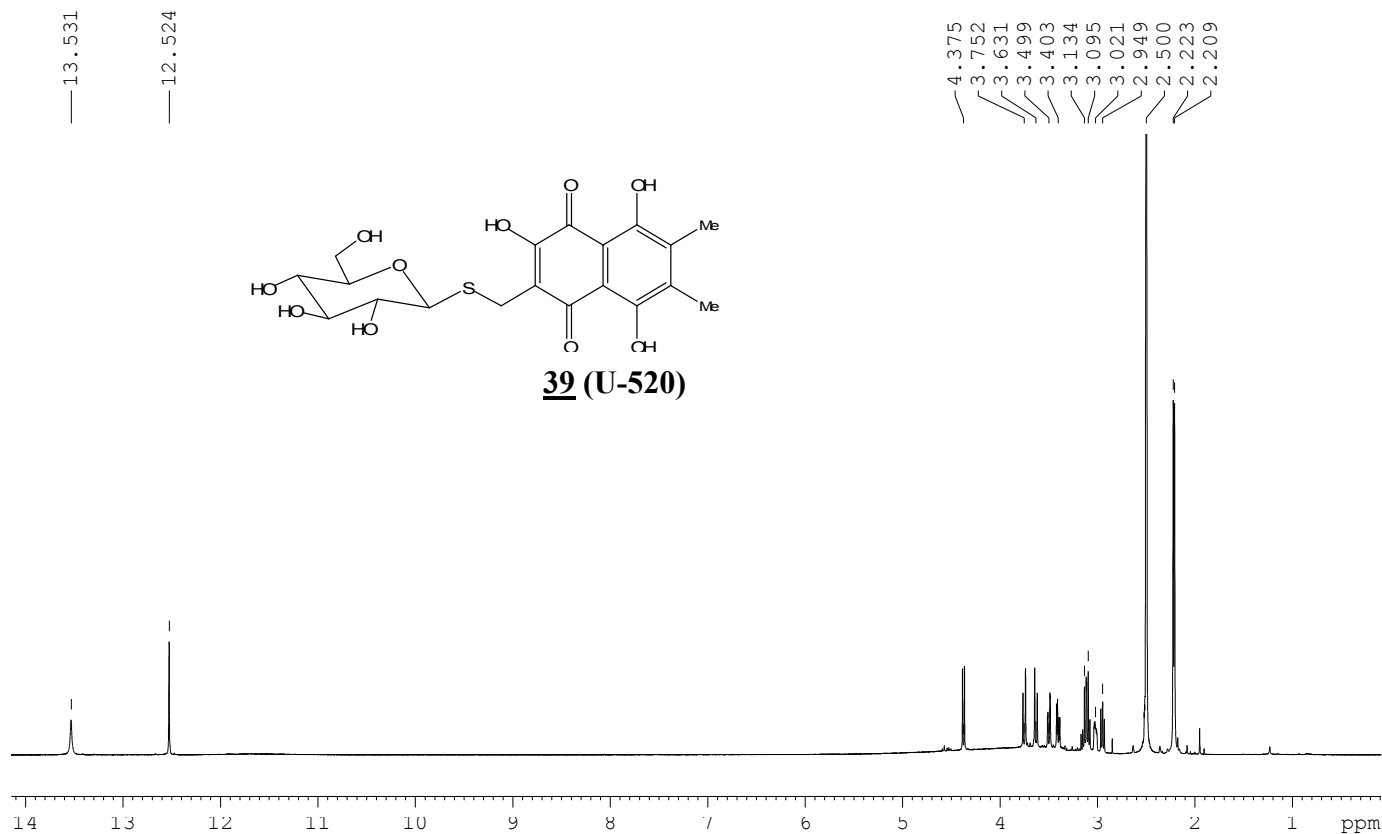
3-(Tetra-O-acetyl- β -D-glucopyranosyl-1-thiomethyl)-2,5,8-trihydroxy-6,7-dimethoxynaphthalene-1,4-dione **32** (U-637), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



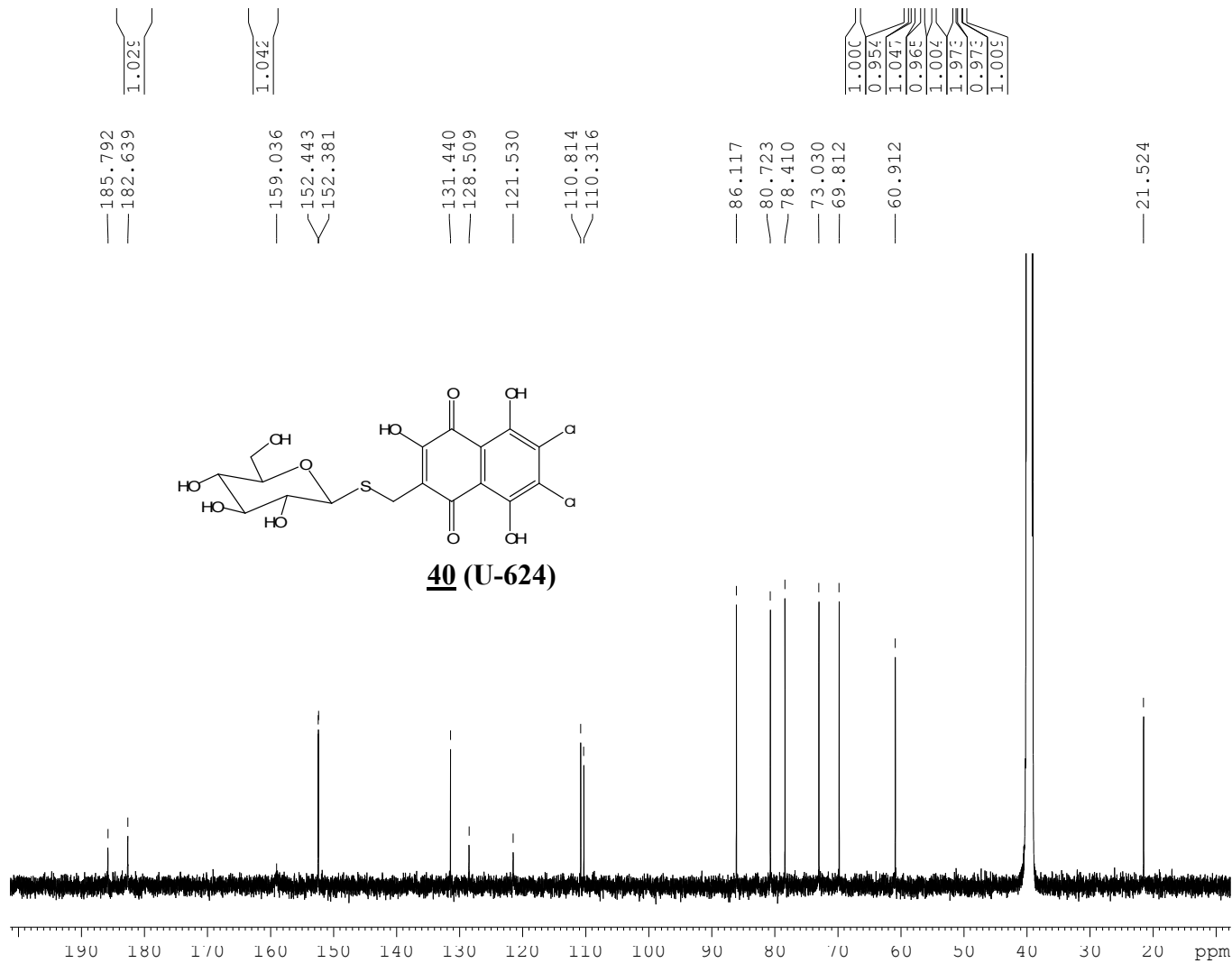
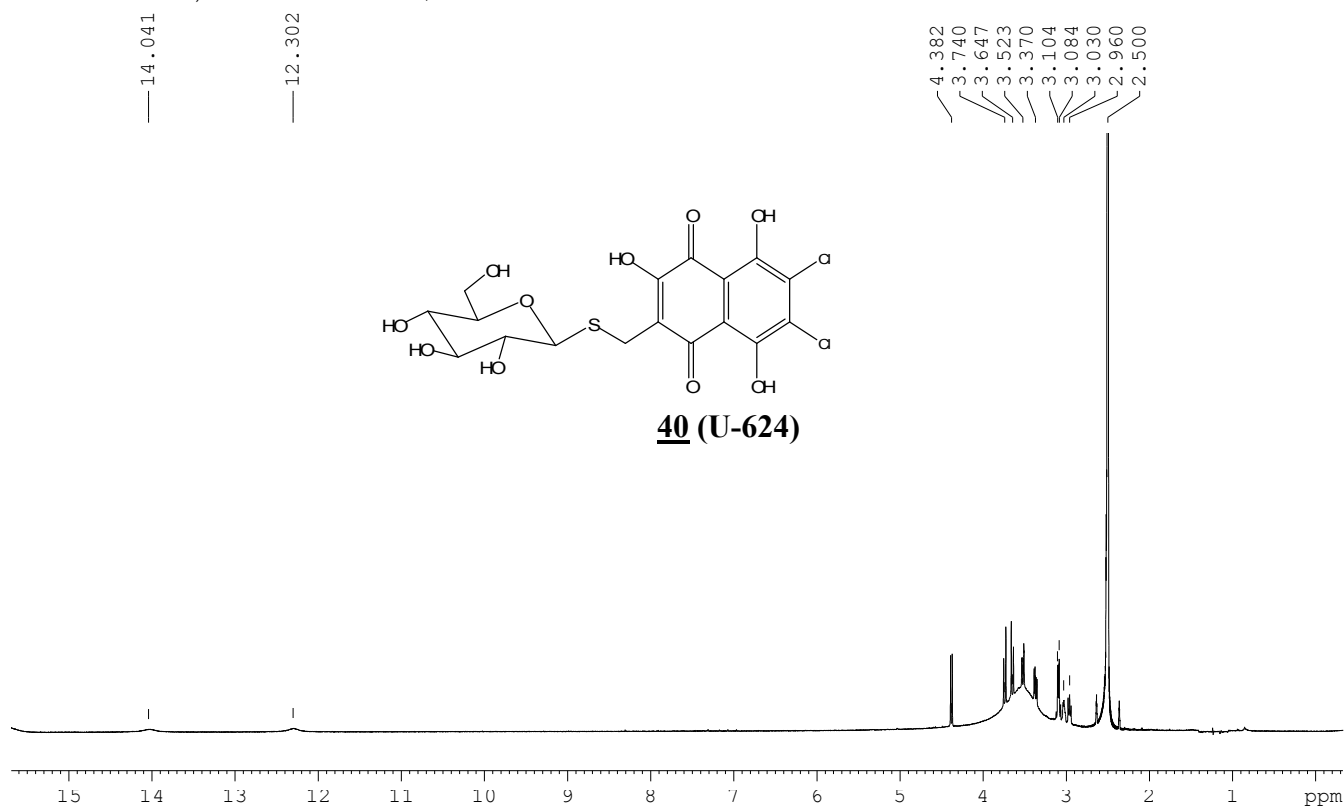
3-(β -D-Glucopyranosyl-1-thiomethyl)-2,5,8-trihydroxynaphthalene-1,4-dione **38** (U-635), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



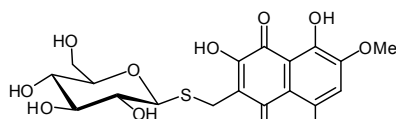
3-(β -D-Glucopyranosyl-1-thiomethyl)-2,5,8-trihydroxy-6,7-dimethylnaphthalene-1,4-dione **39** (U-520), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



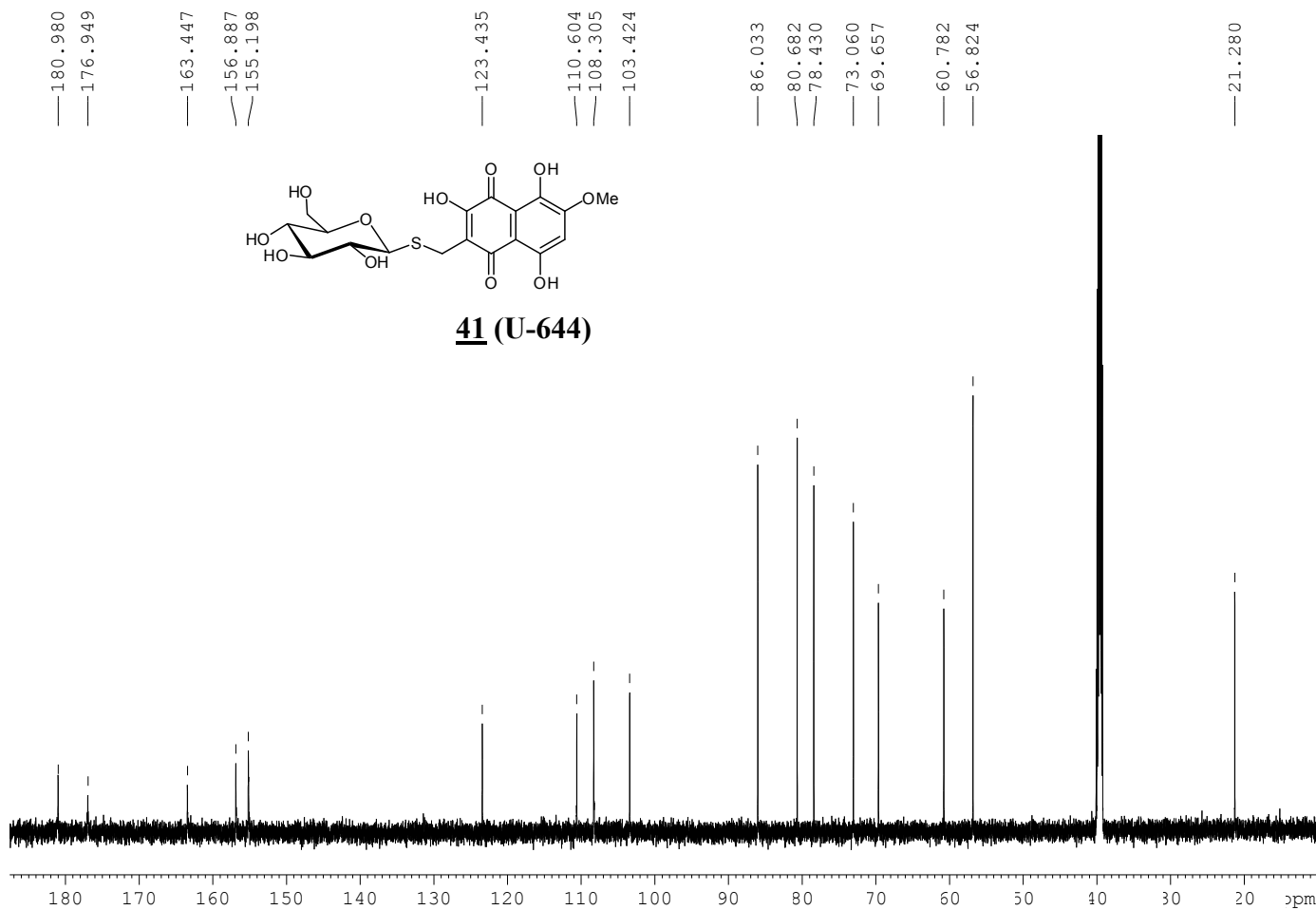
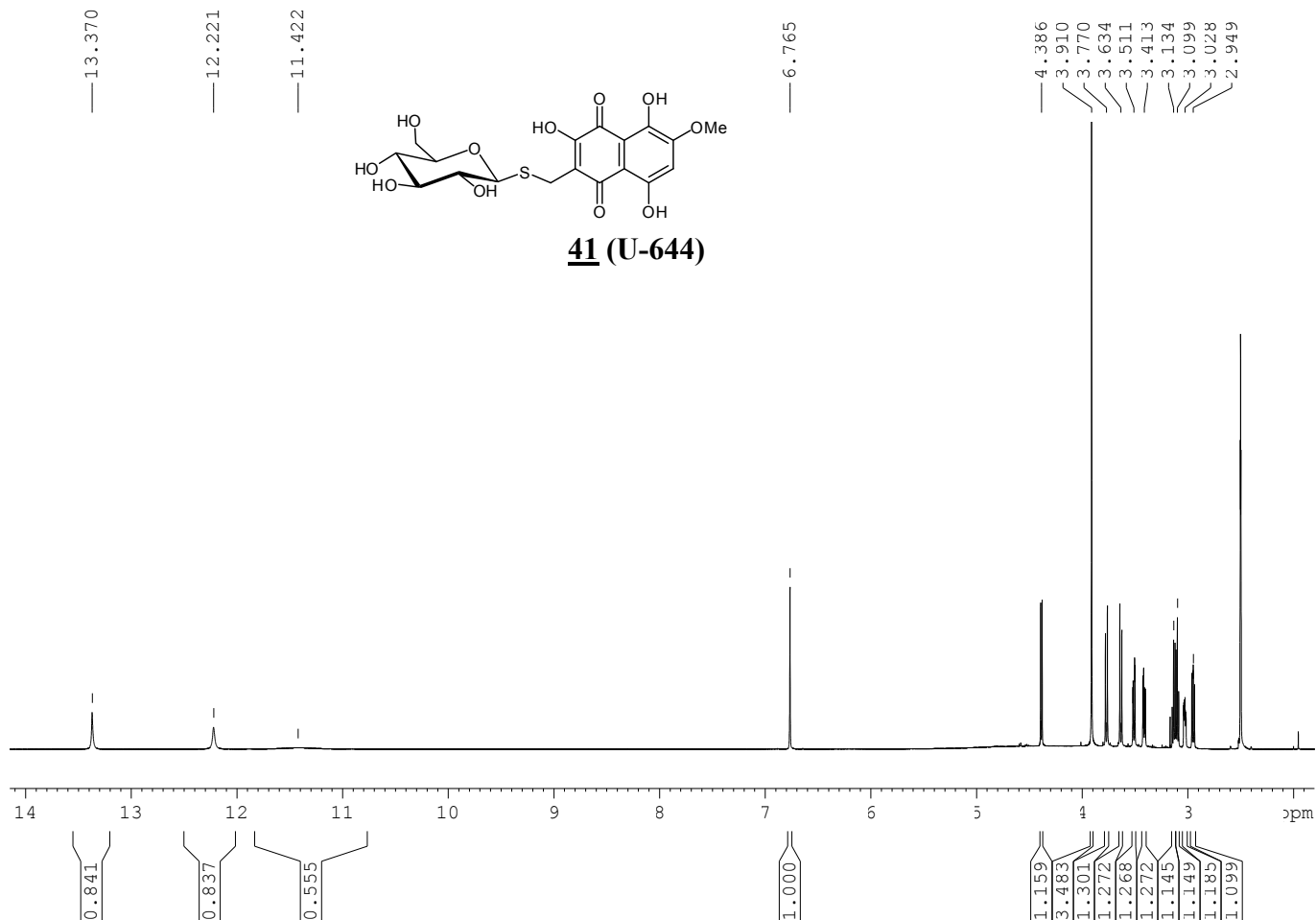
6,7-Dichloro-3-(β -D-glucopyranosyl-1-thiomethyl)-2,5,8-trihydroxynaphthalene-1,4-dione **40** (U-624), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



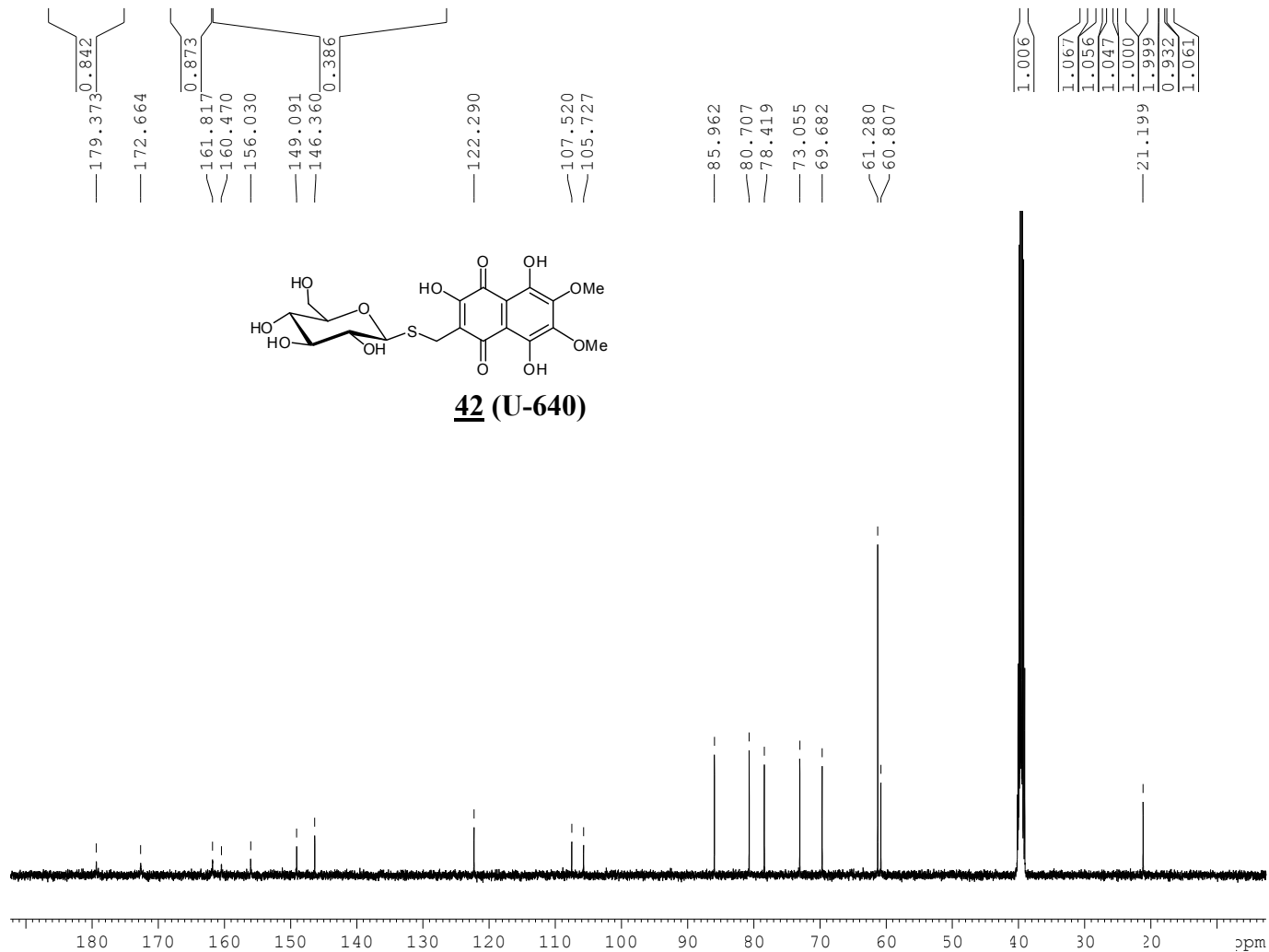
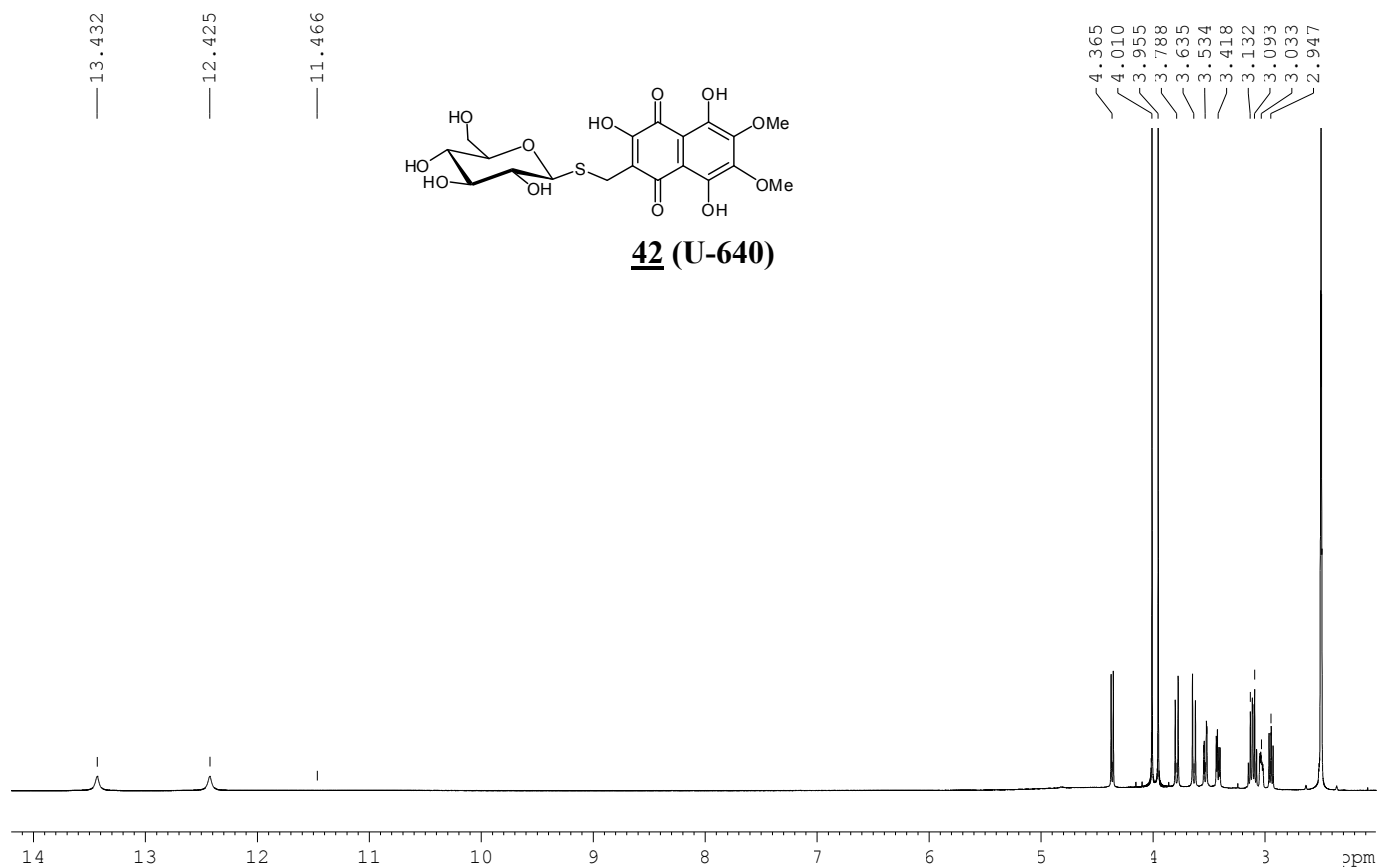
3-(β -D-Glucopyranosyl-1-thiomethyl)-2,5,8-trihydroxy-7-methoxynaphthalene-1,4-dione **41** (U-644), (^1H NMR - 700 MHz, ^{13}C NMR - 176 MHz, solvent - DMSO- d_6)



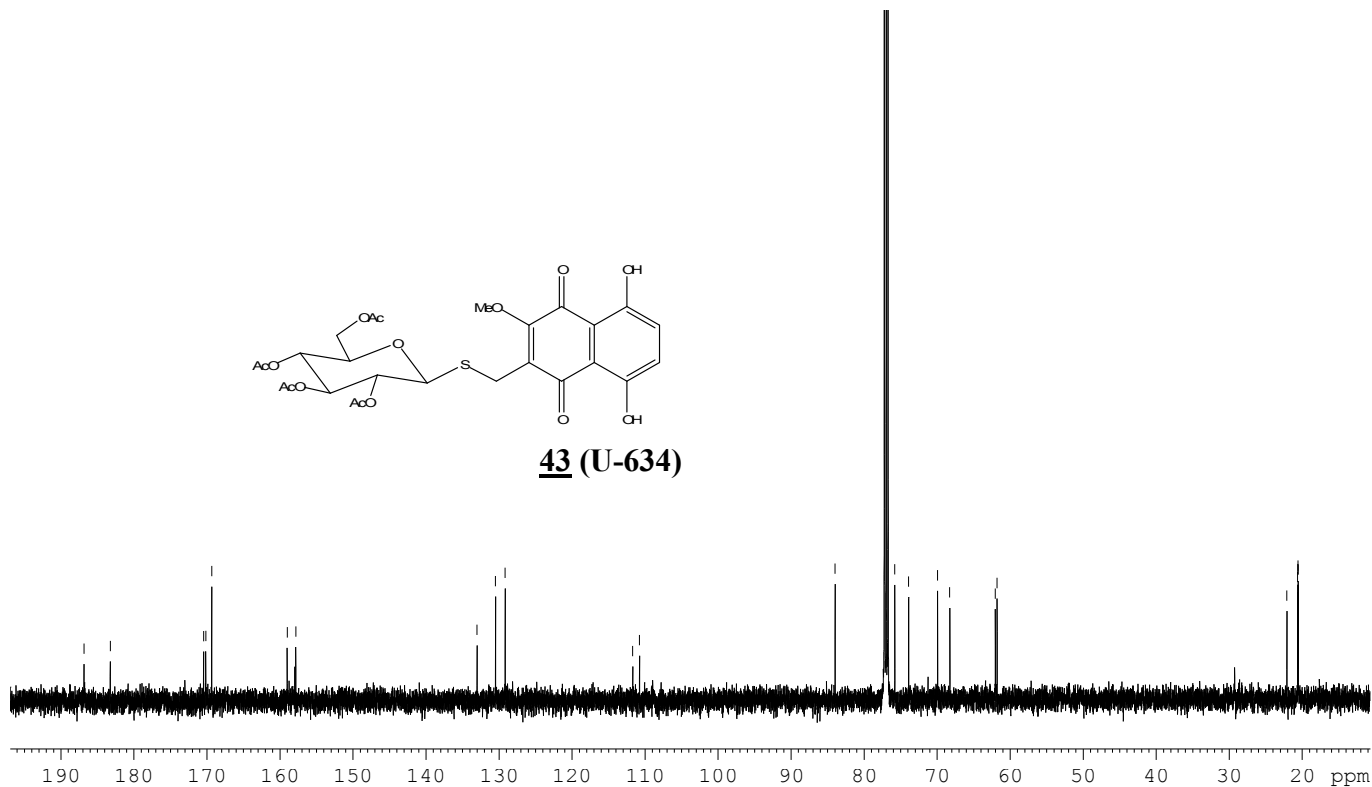
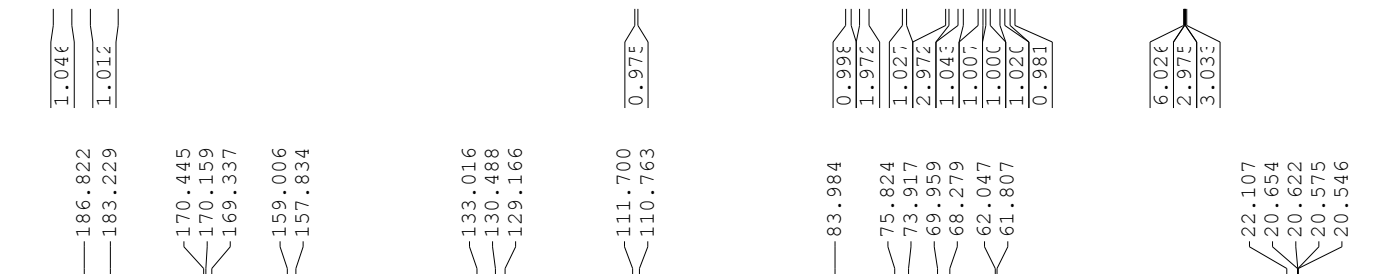
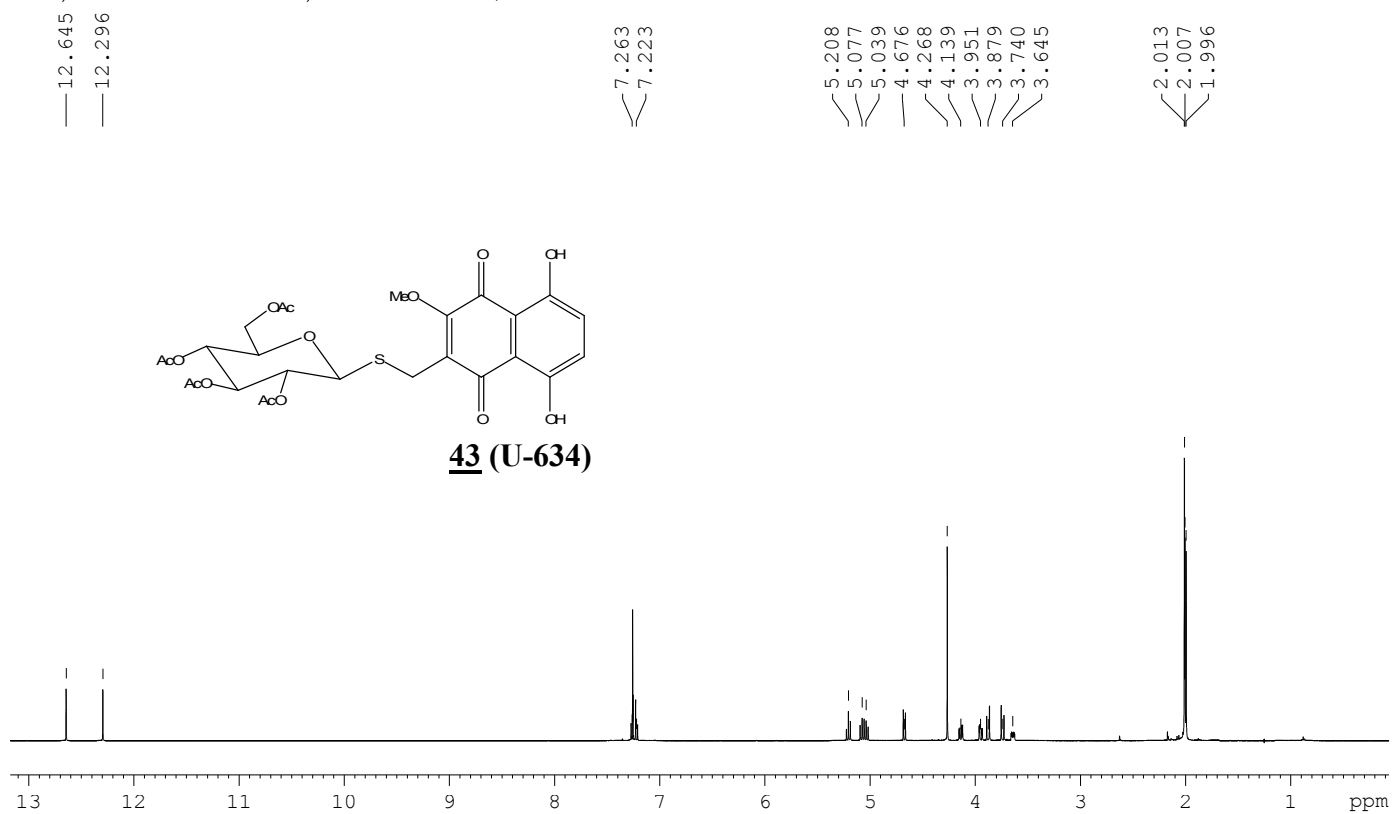
41 (U-644)



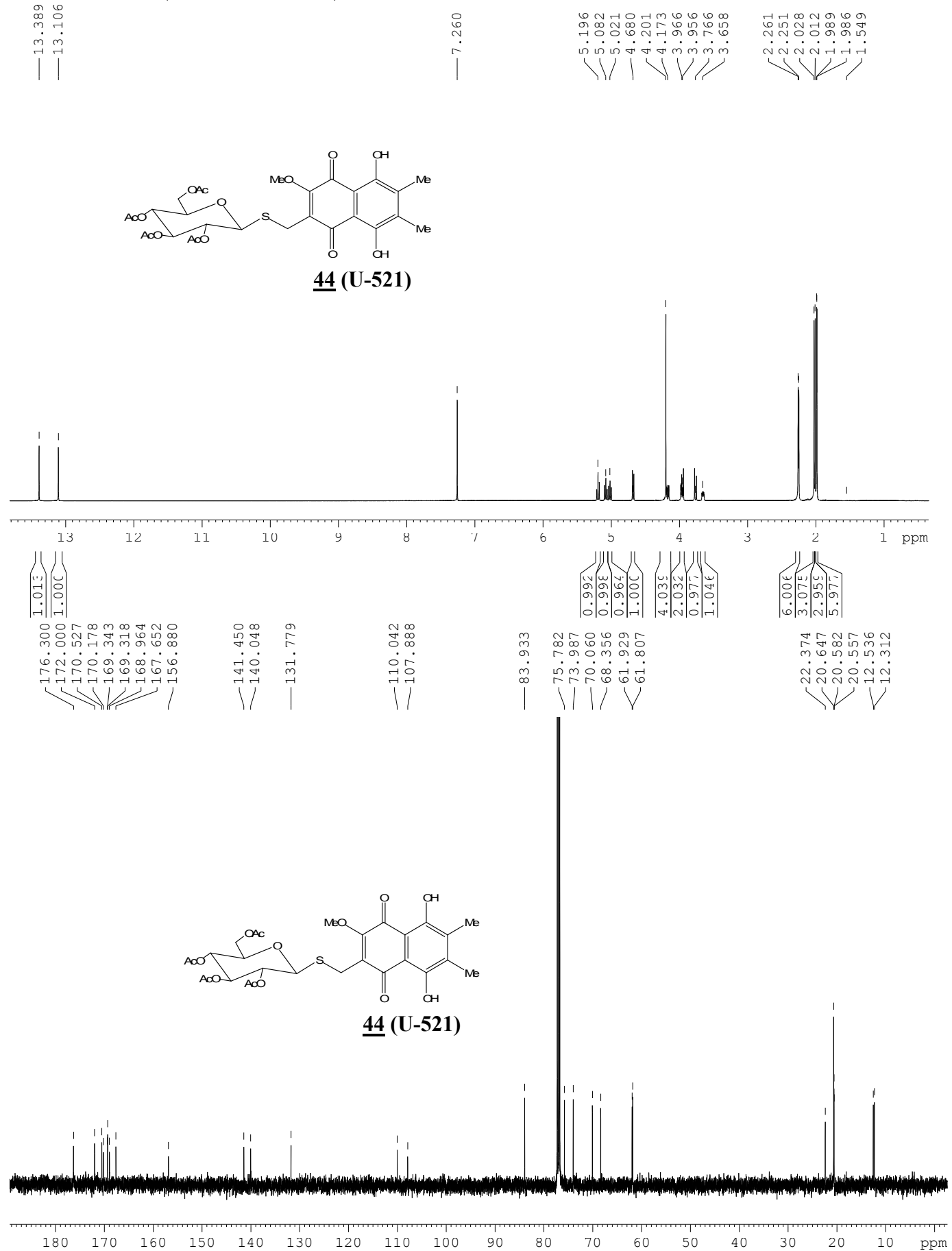
3-(β -D-Glucopyranosyl-1-thiomethyl)-2,5,8-trihydroxy-6,7-dimethoxynaphthalene-1,4-dione **42** (U-640), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



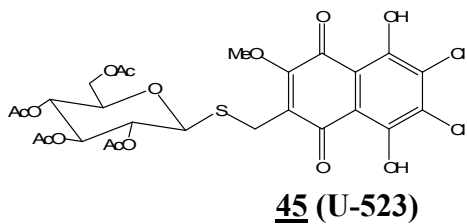
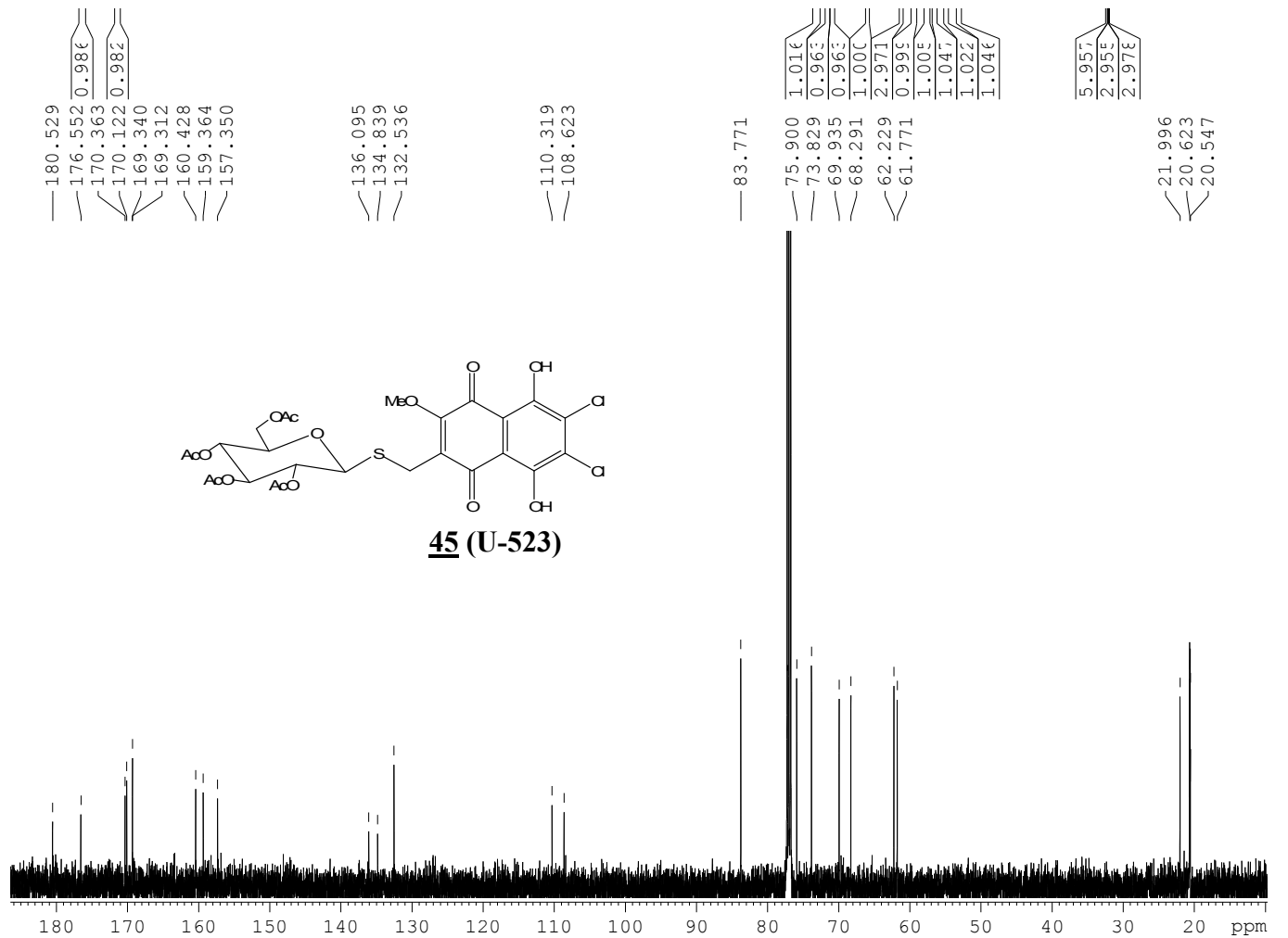
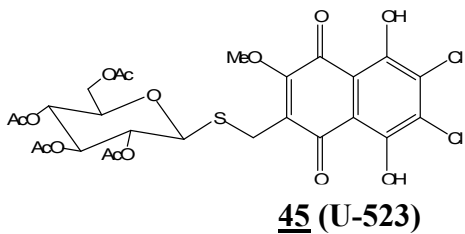
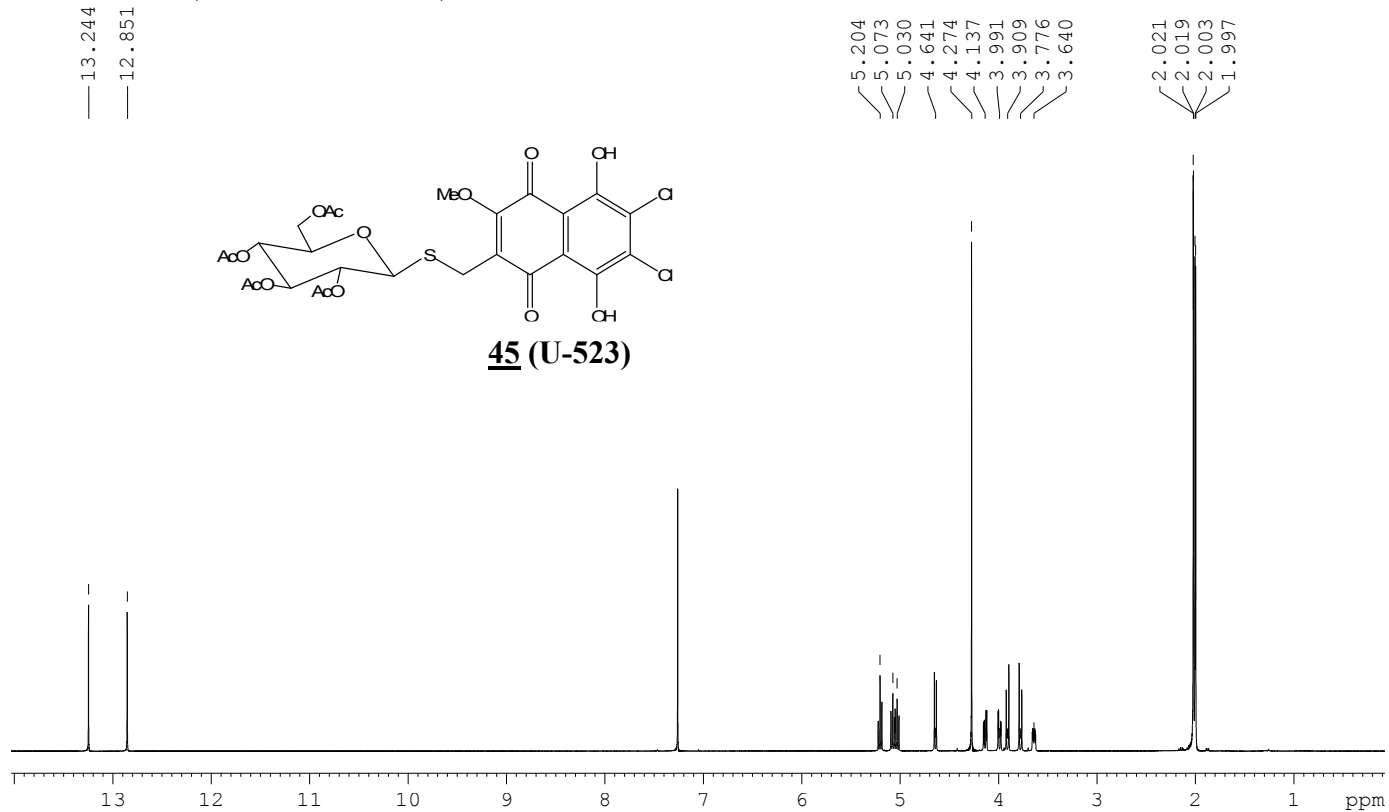
3-(Tetra-O-acetyl- β -D-glucopyranosyl-1-thiomethyl)-5,8-dihydroxy-2-methoxynaphthalene-1,4-dione **43** (U-634), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



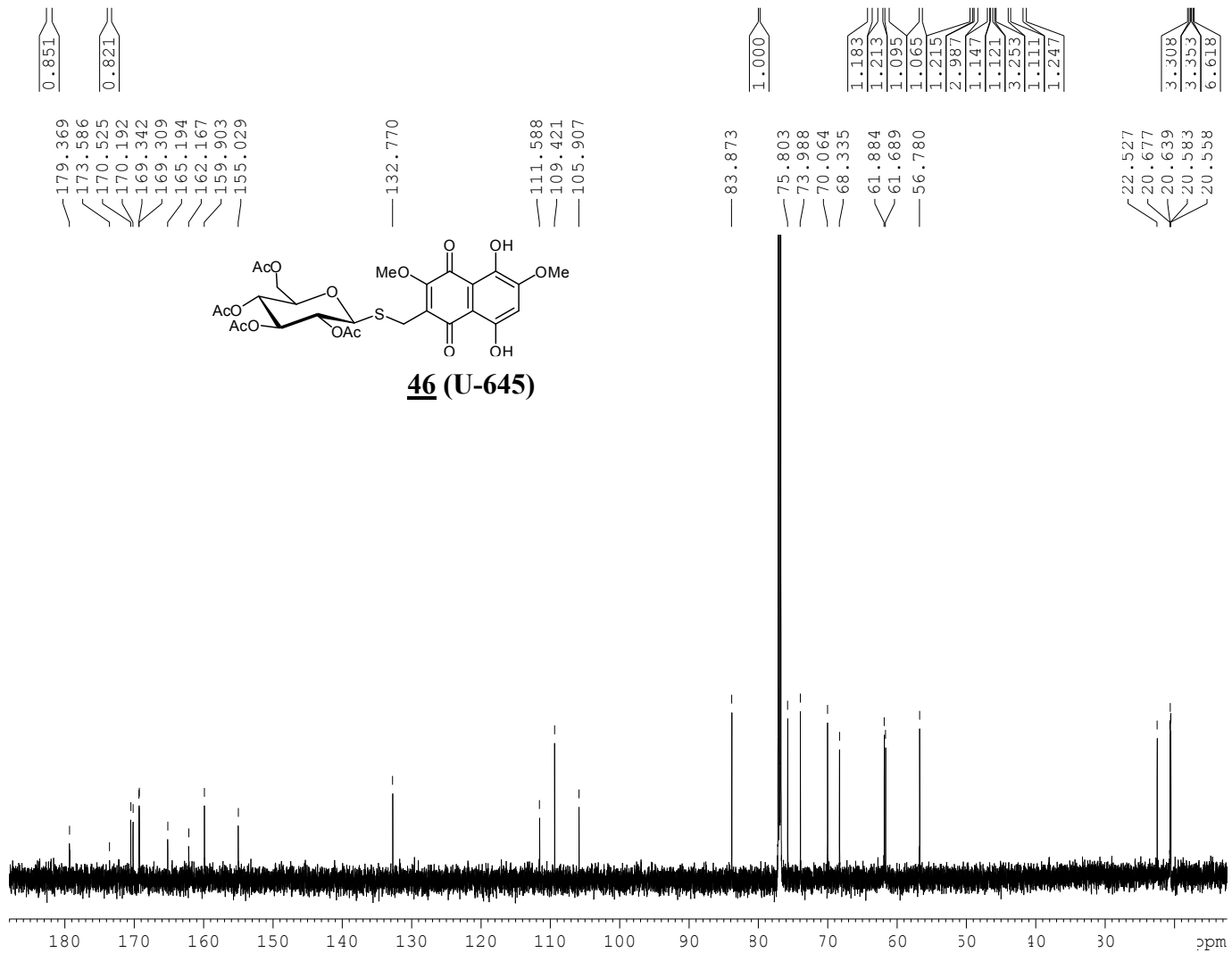
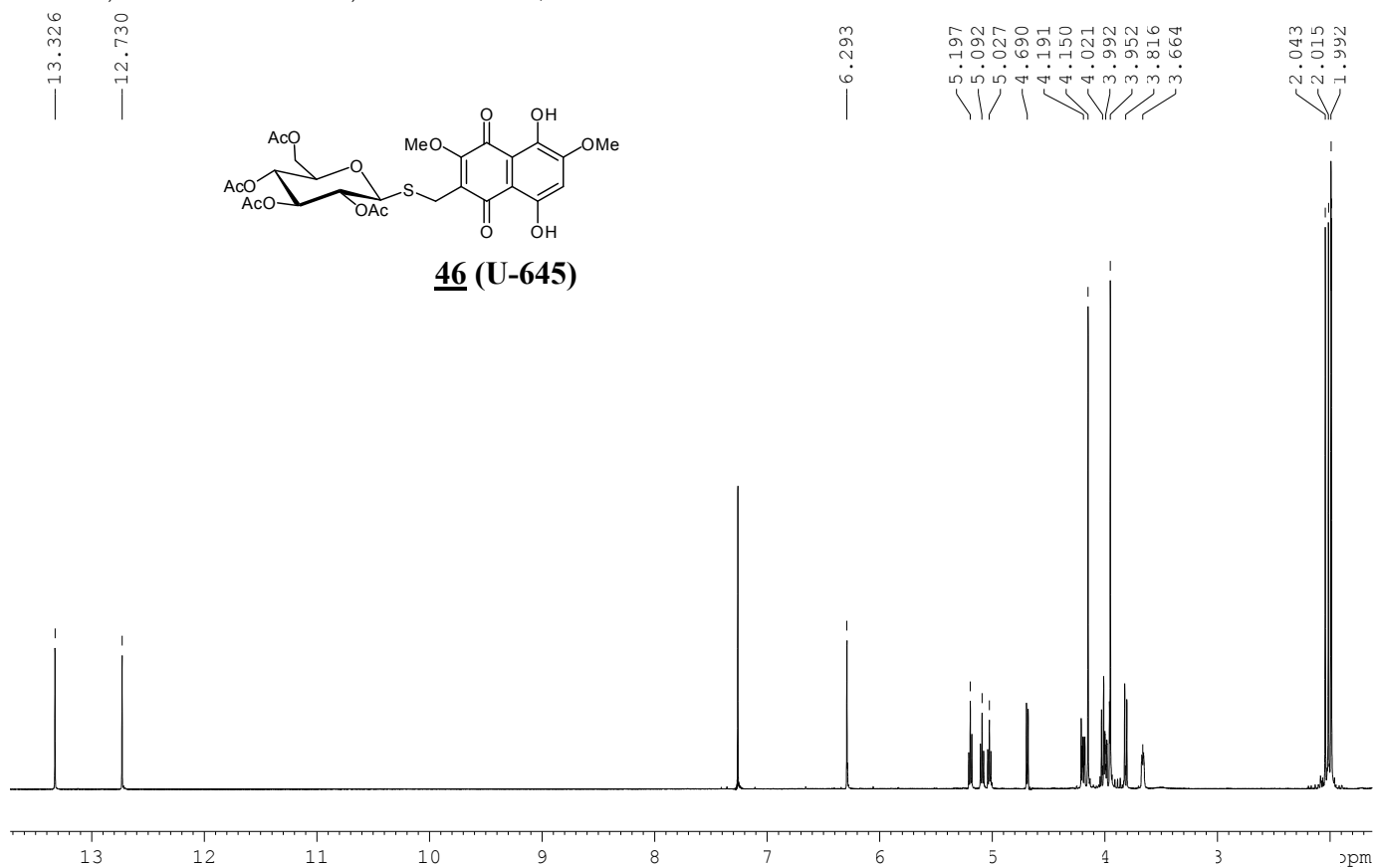
3-(Tetra-O-acetyl- β -D-glucopyranosyl-1-thiomethyl)-5,8-dihydroxy-2-methoxy-6,7-dimethylnaphthalene-1,4-dione **44** (U-521),
 (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



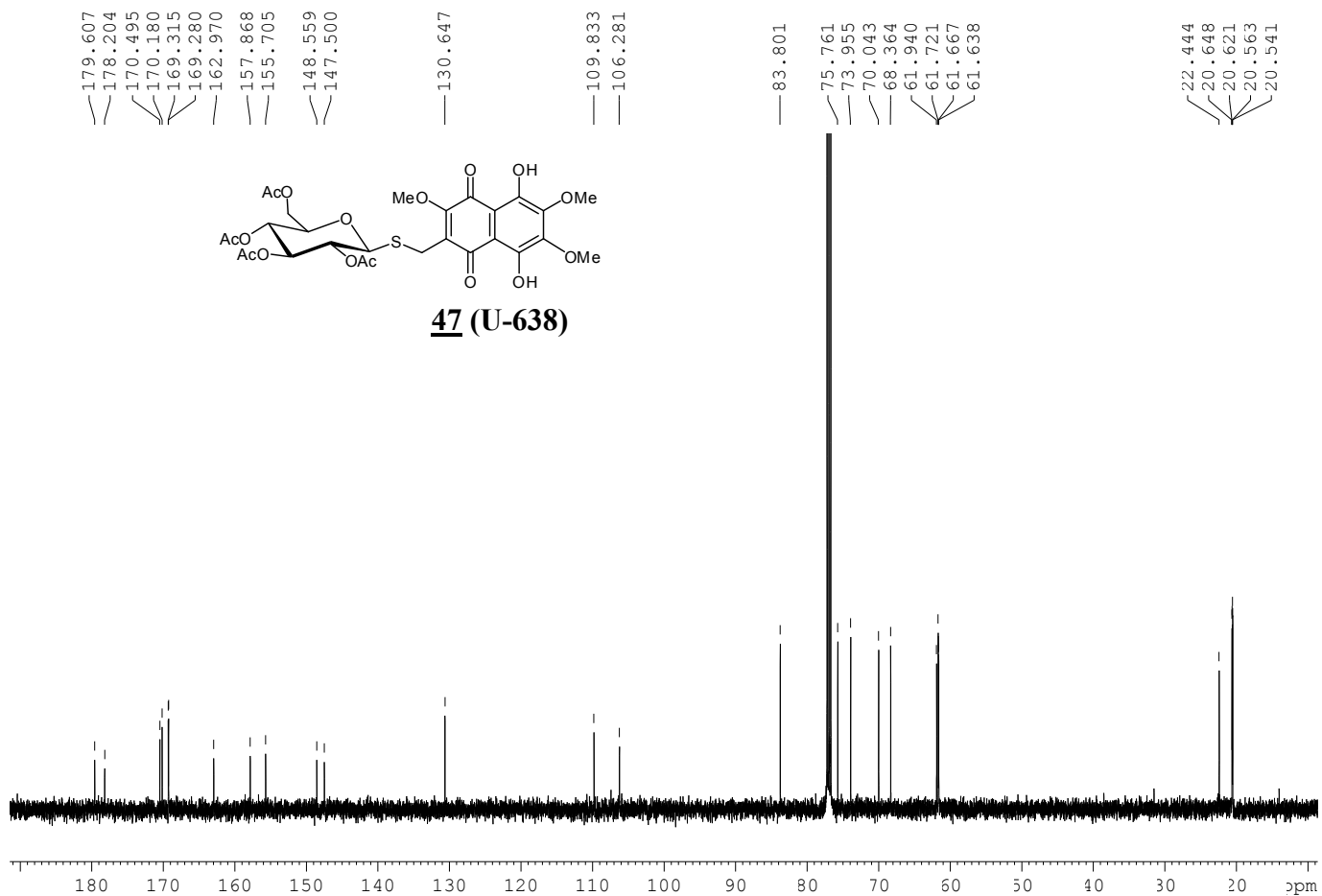
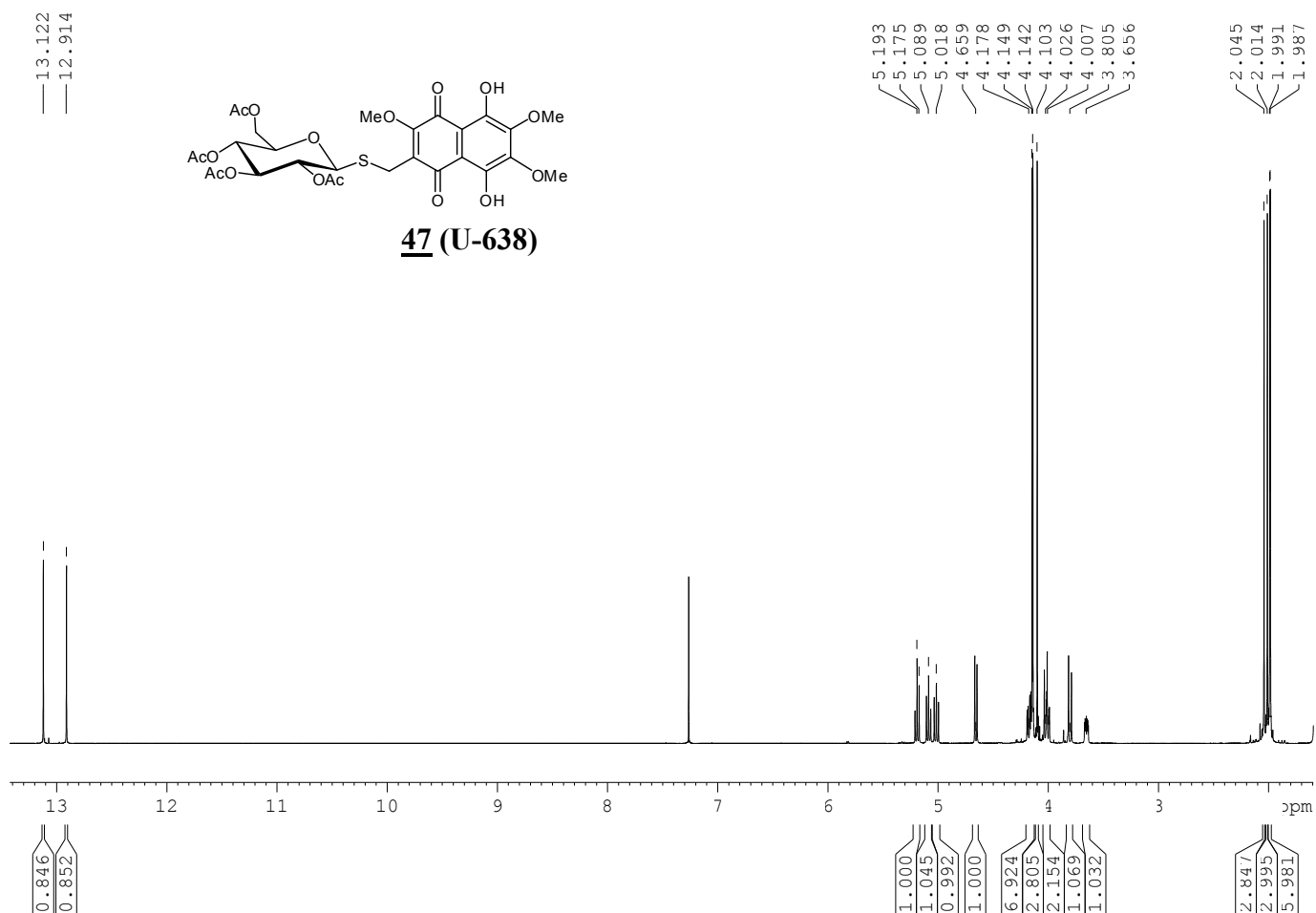
3-(Tetra-O-acetyl-β-D-glucopyranosyl-1-thiomethyl)-6,7-dichloro-5,8-dihydroxy-2-methoxynaphthalene-1,4-dione **45** (U-523), (¹H NMR - 500 MHz, ¹³C NMR - 125 MHz, solvent – CDCl₃)



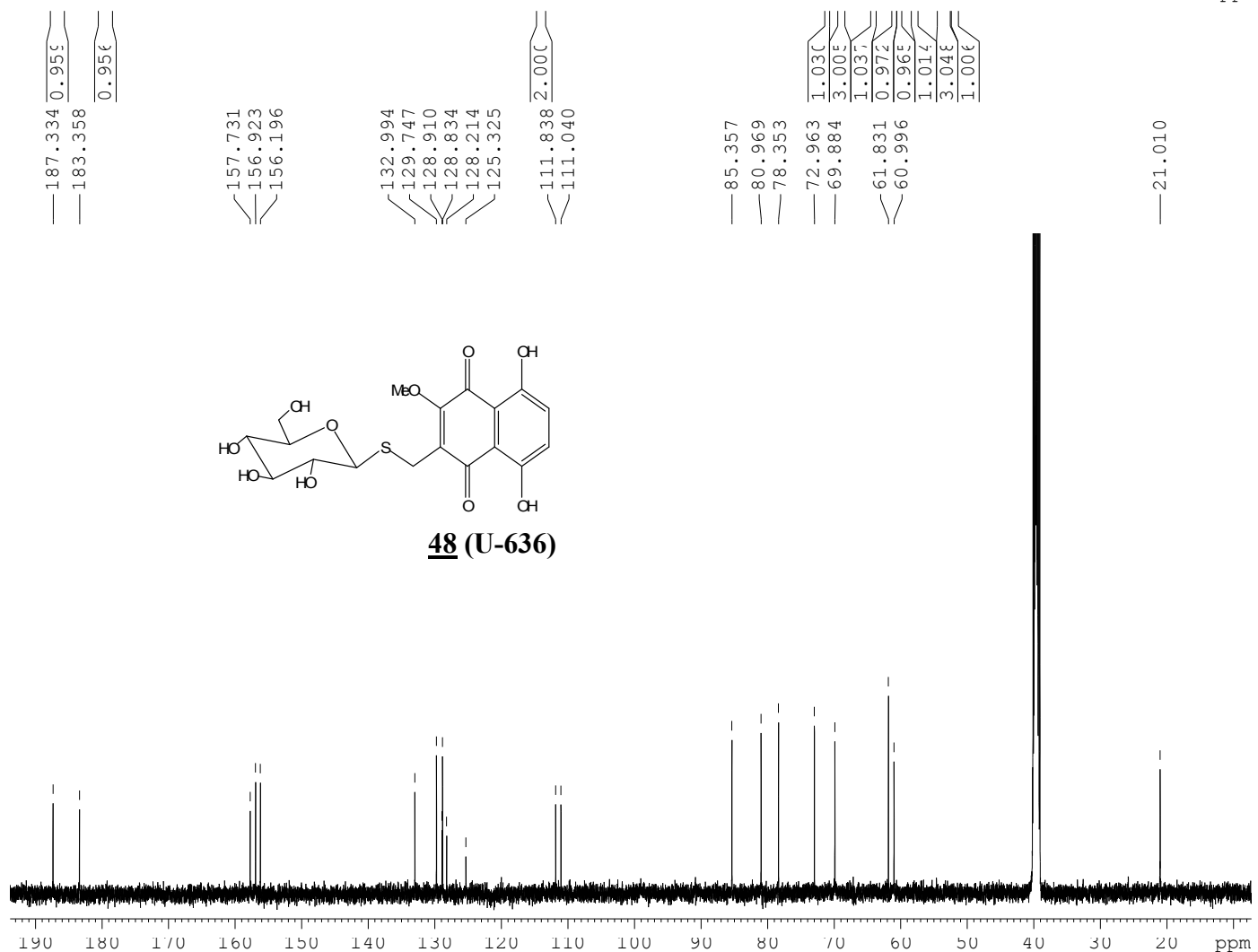
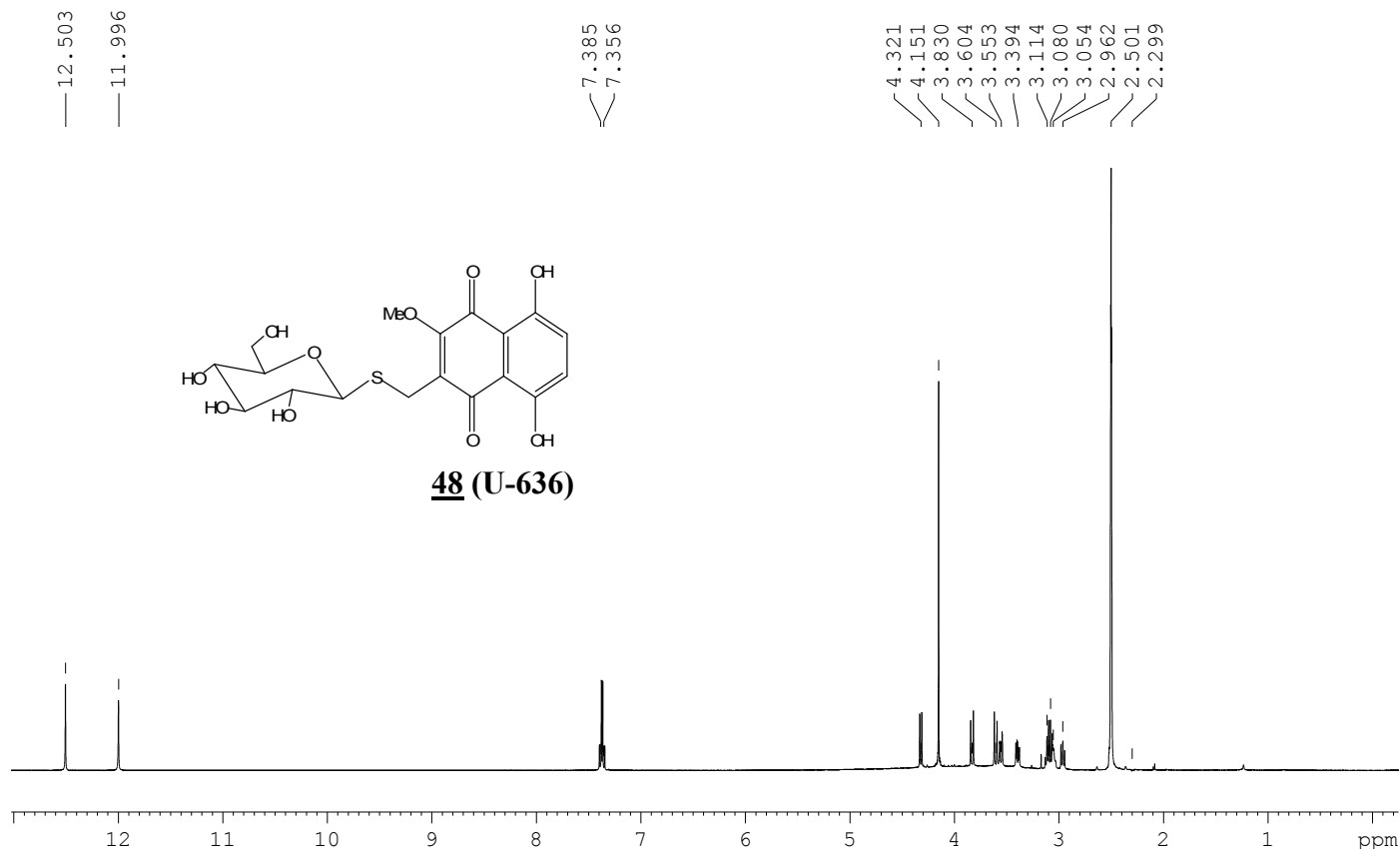
3-(Tetra-O-acetyl- β -D-glucopyranosyl-1-thiomethyl)-5,8-dihydroxy-2,7-dimethoxynaphthalene-1,4-dione **46** (U-645), (^1H NMR - 700 MHz, ^{13}C NMR - 176 MHz, solvent - CDCl_3)



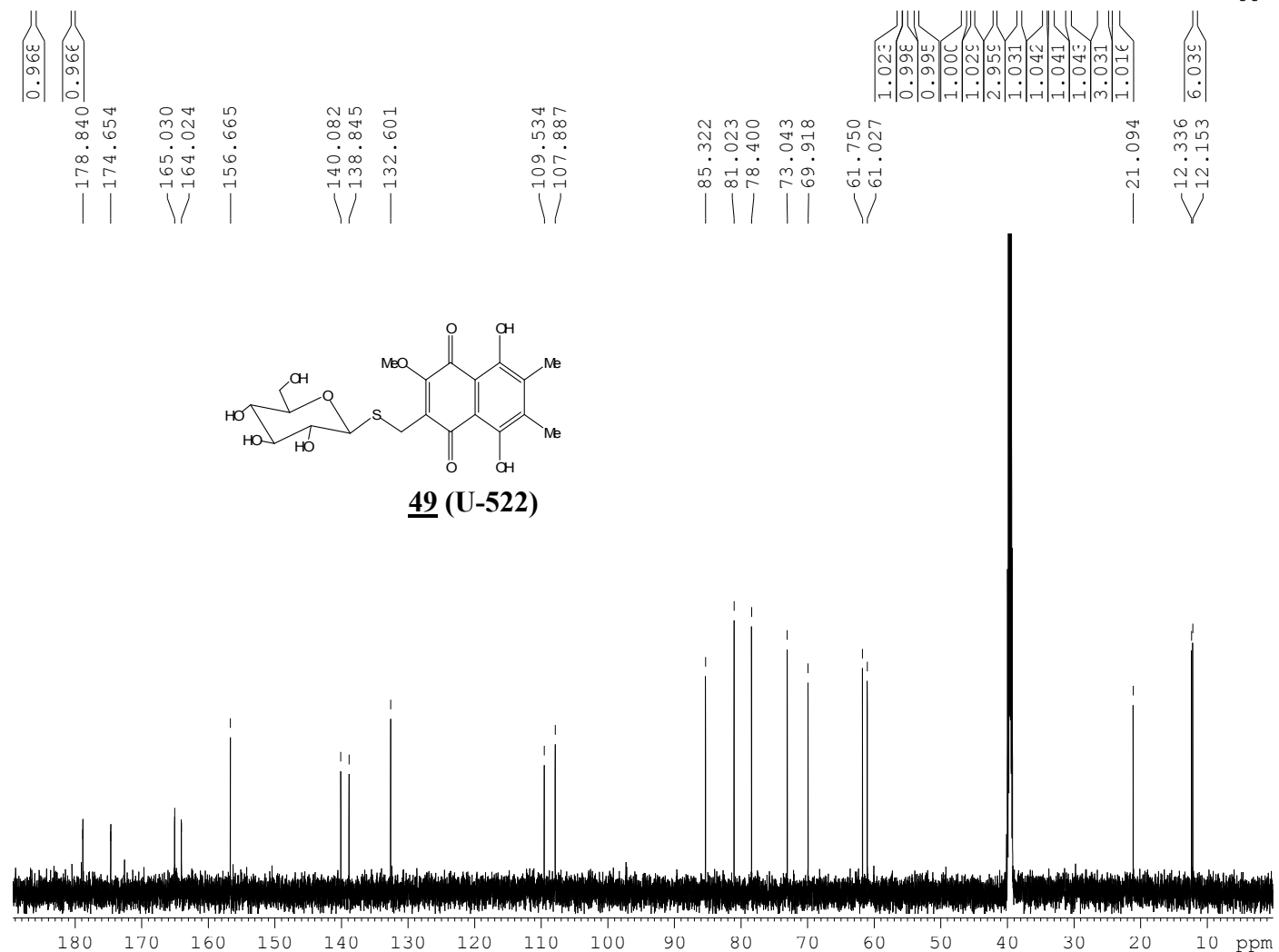
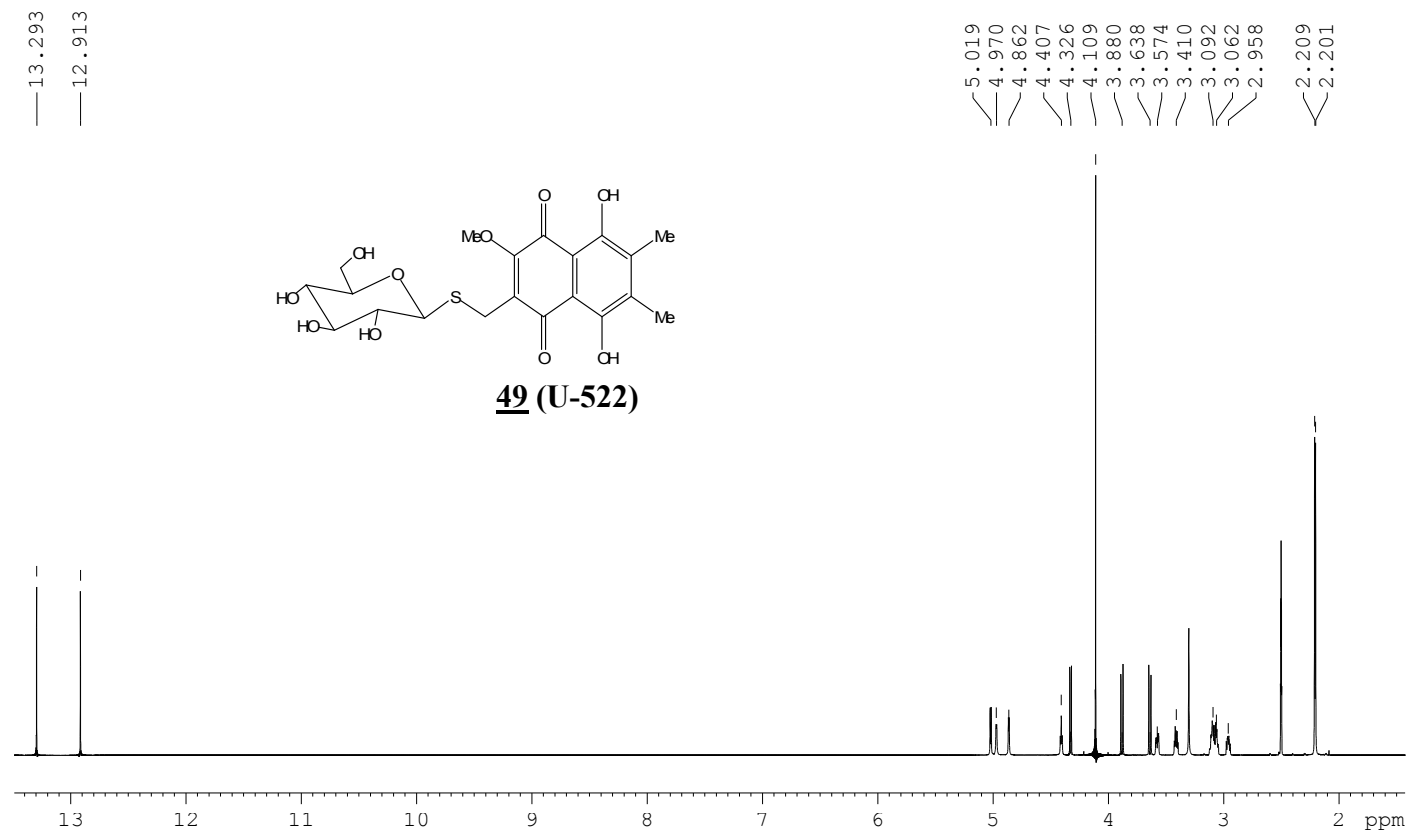
3-(Tetra-O-acetyl-β-D-glucopyranosyl-1-thiomethyl)-5,8-dihydroxy-2,6,7-trimethoxynaphthalene-1,4-dione **47** (U-638), (¹H NMR - 500 MHz, ¹³C NMR - 125 MHz, solvent – CDCl₃)



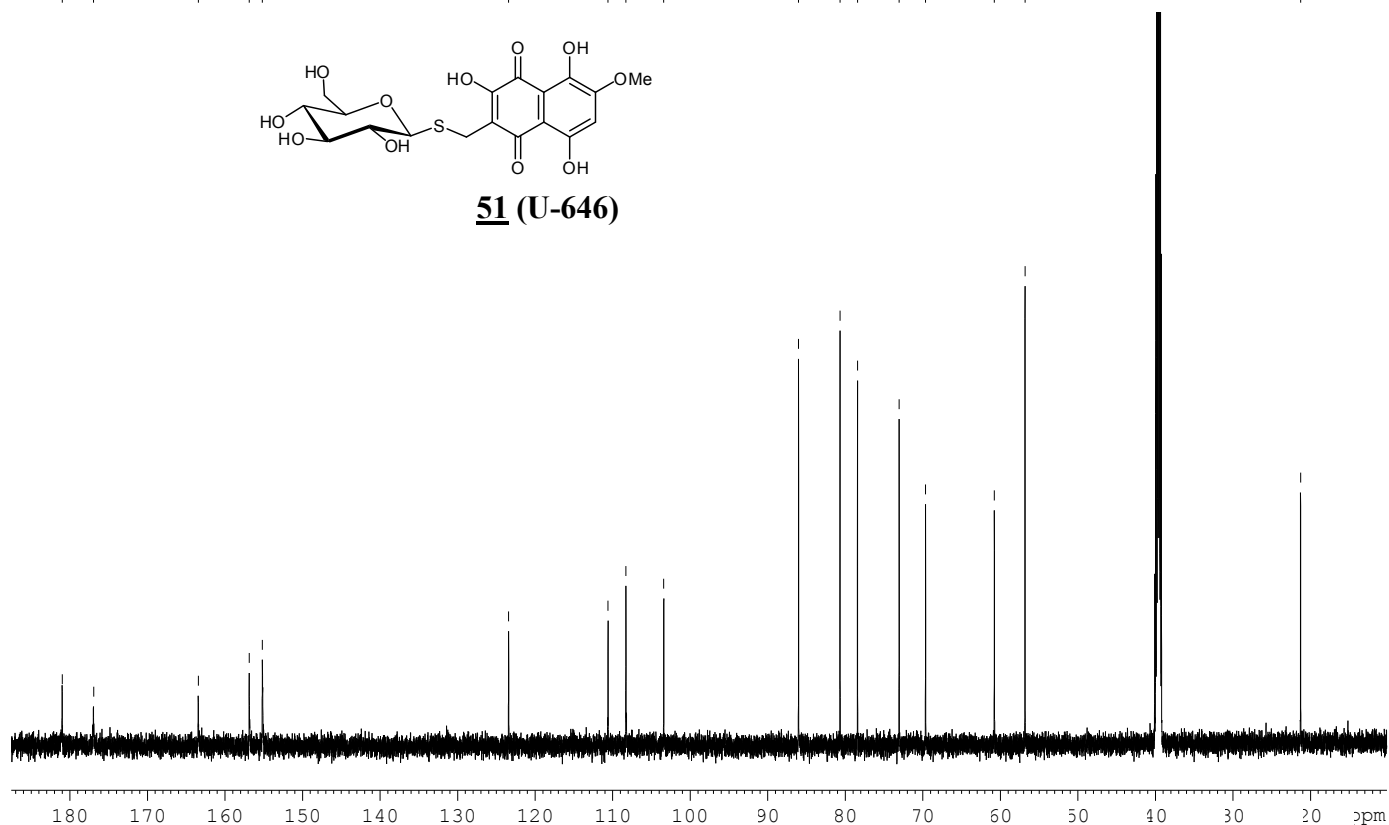
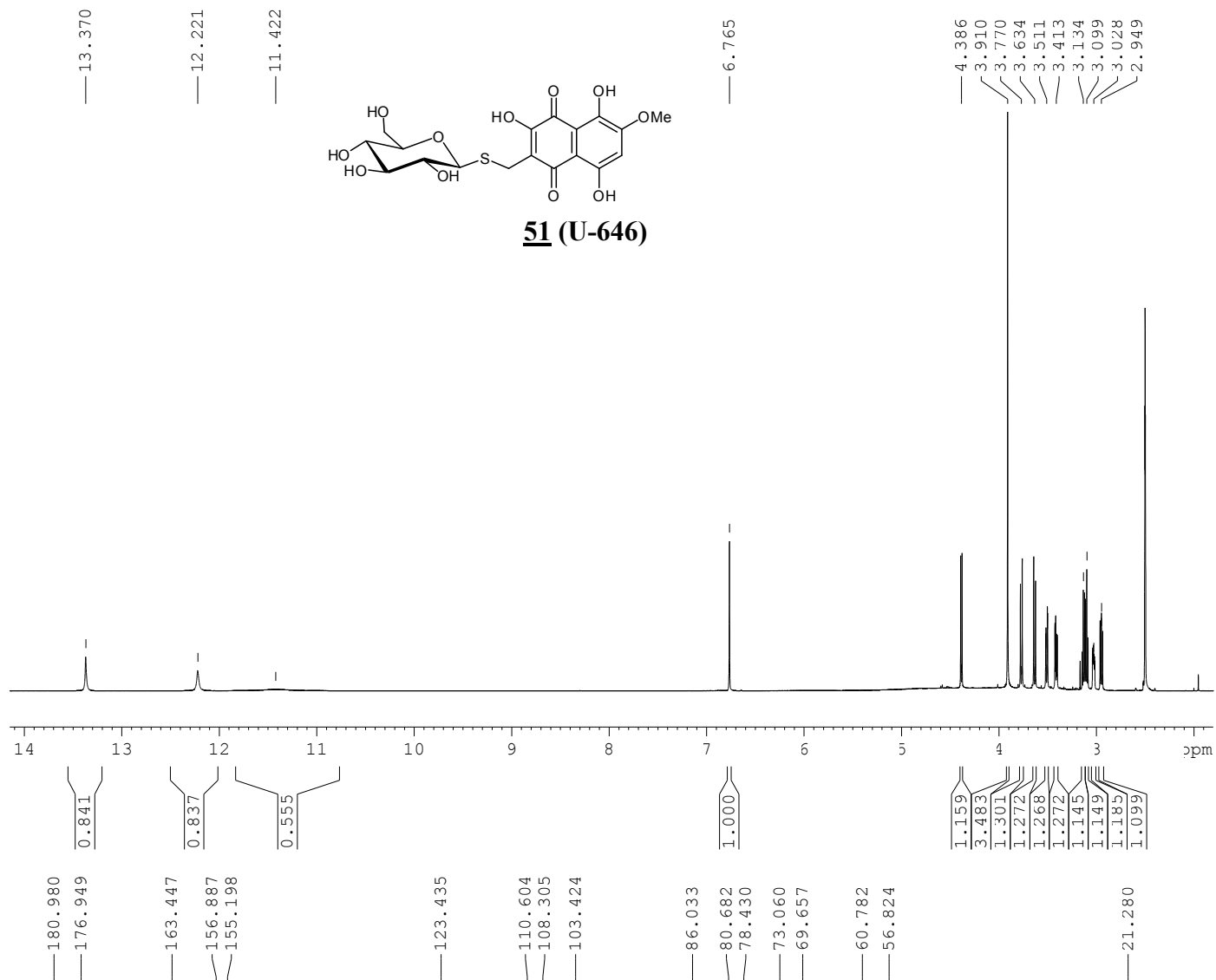
3-(β -D-Glucopyranosyl-1-thiomethyl)-5,8-dihydroxy-3-methoxynaphthalene-1,4-dione **48** (U-636), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



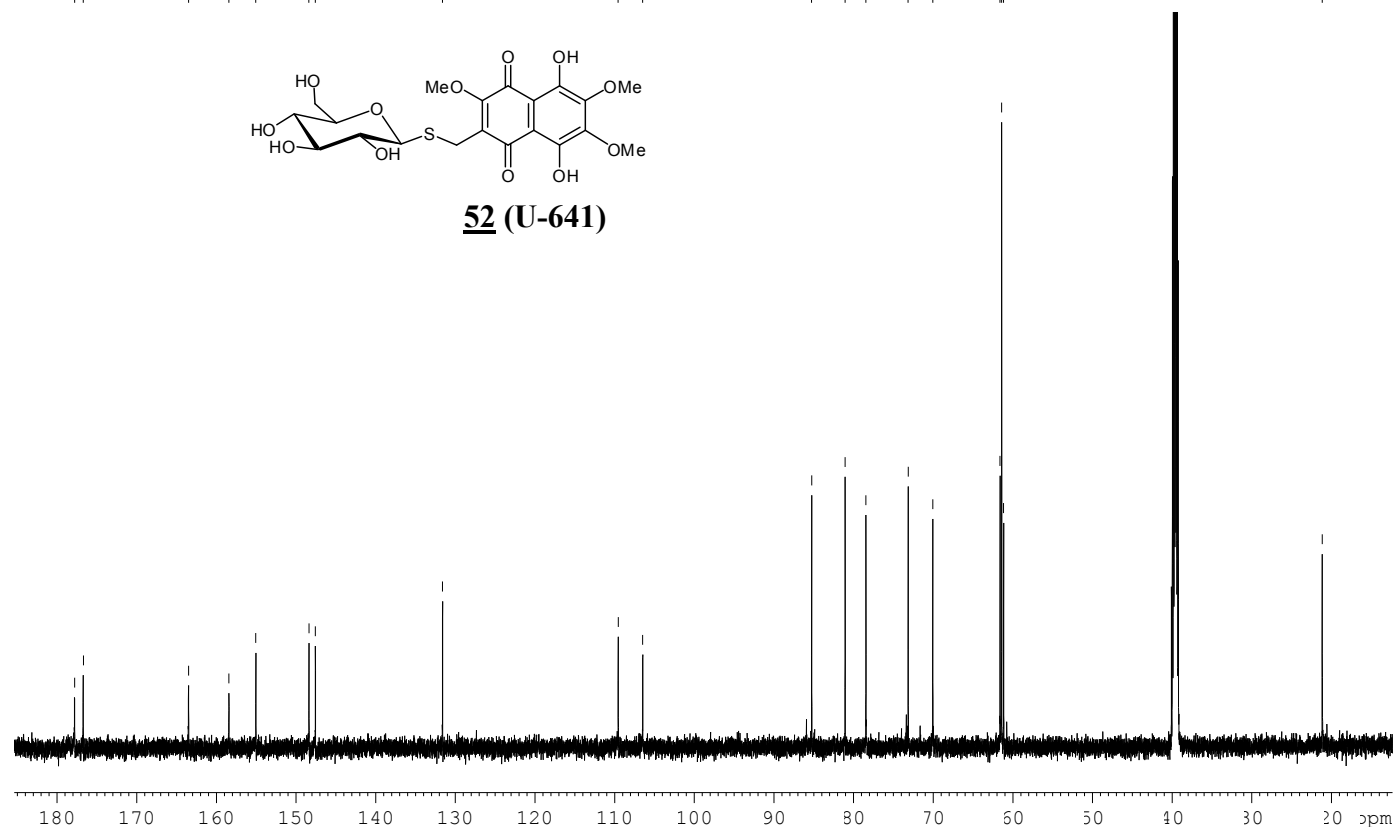
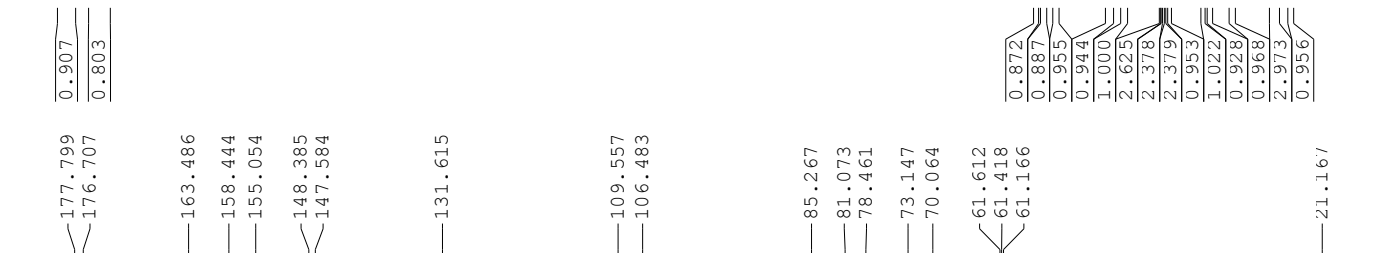
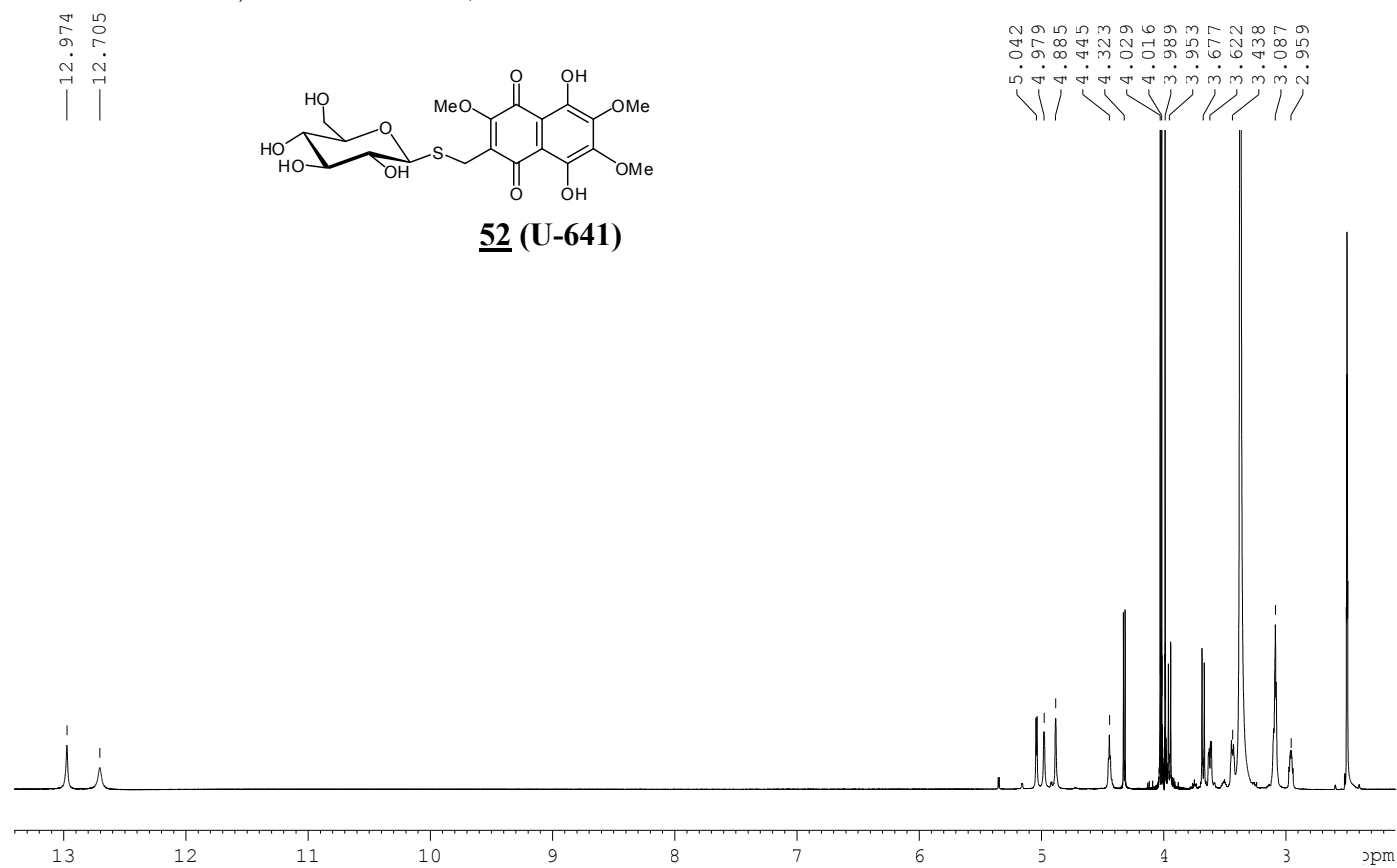
3-(β -D-Glucopyranosyl-1-thiomethyl)-5,8-dihydroxy-2-methoxy-6,7-dimethylnaphthalene-1,4-dione **49** (U-522), (^1H NMR - 700 MHz, ^{13}C NMR - 176 MHz, solvent - DMSO- d_6)



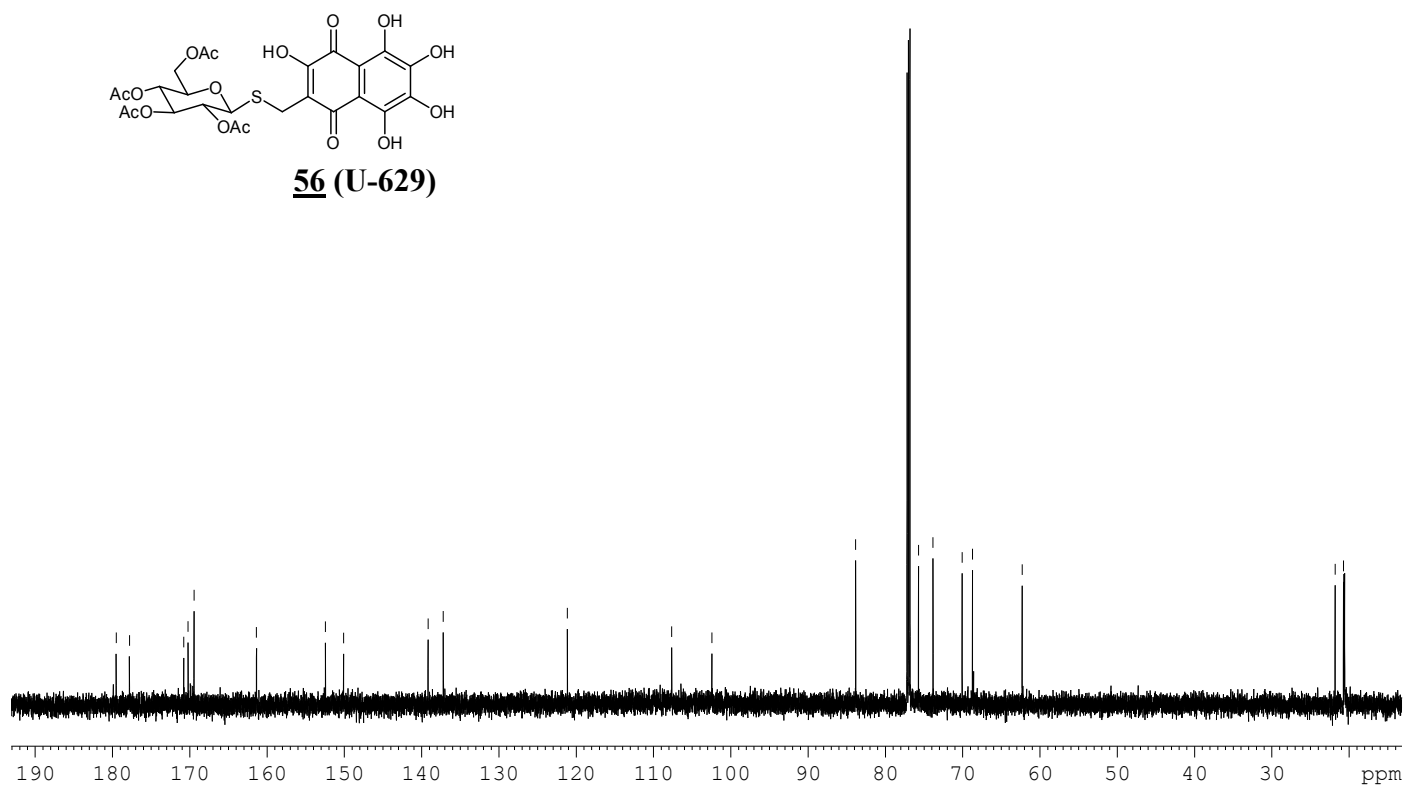
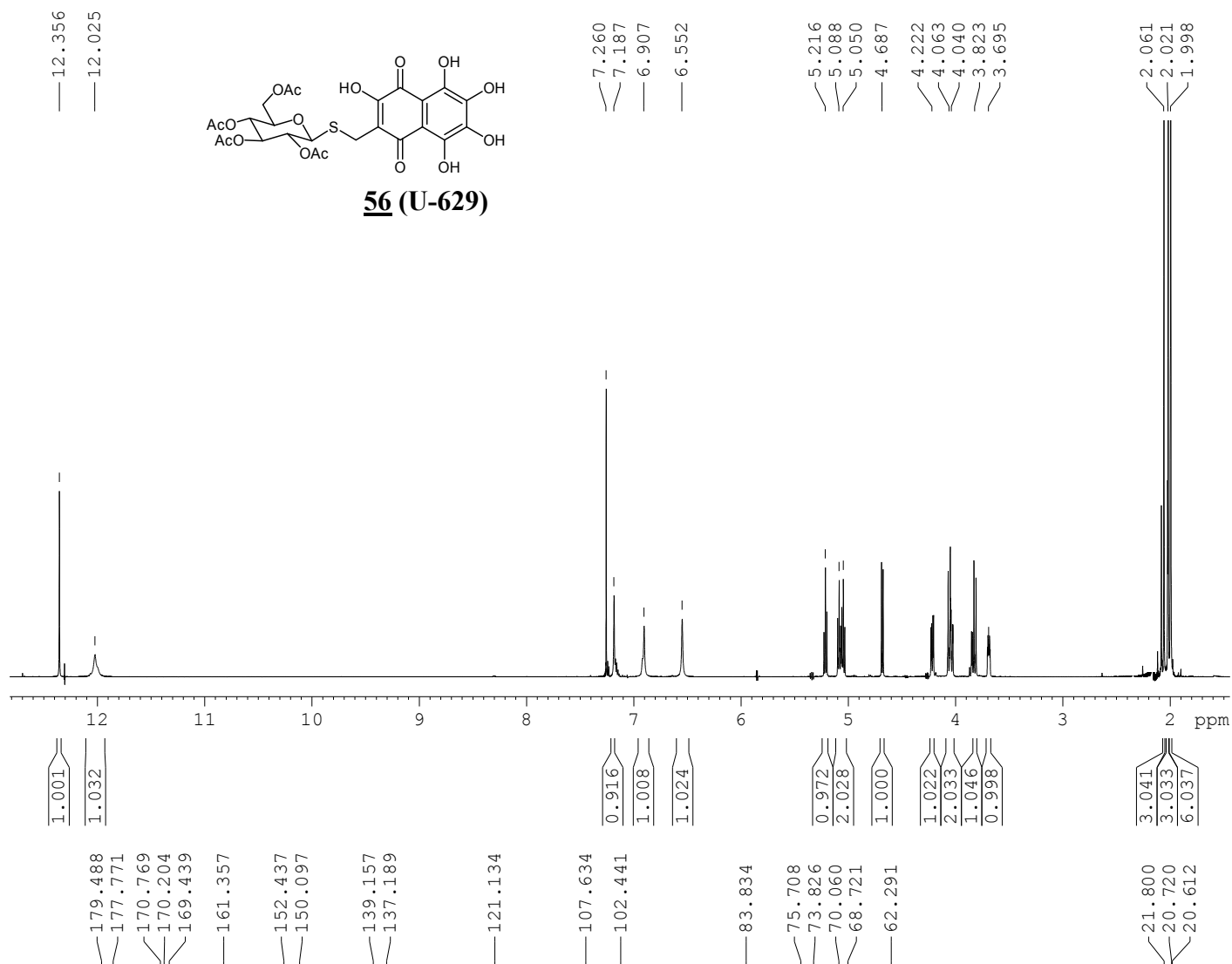
3-(β -D-Glucopyranosyl-1-thiomethyl)-5,8-dihydroxy-2,7-dimethoxynaphthalene-1,4-dione **51** (U-646), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



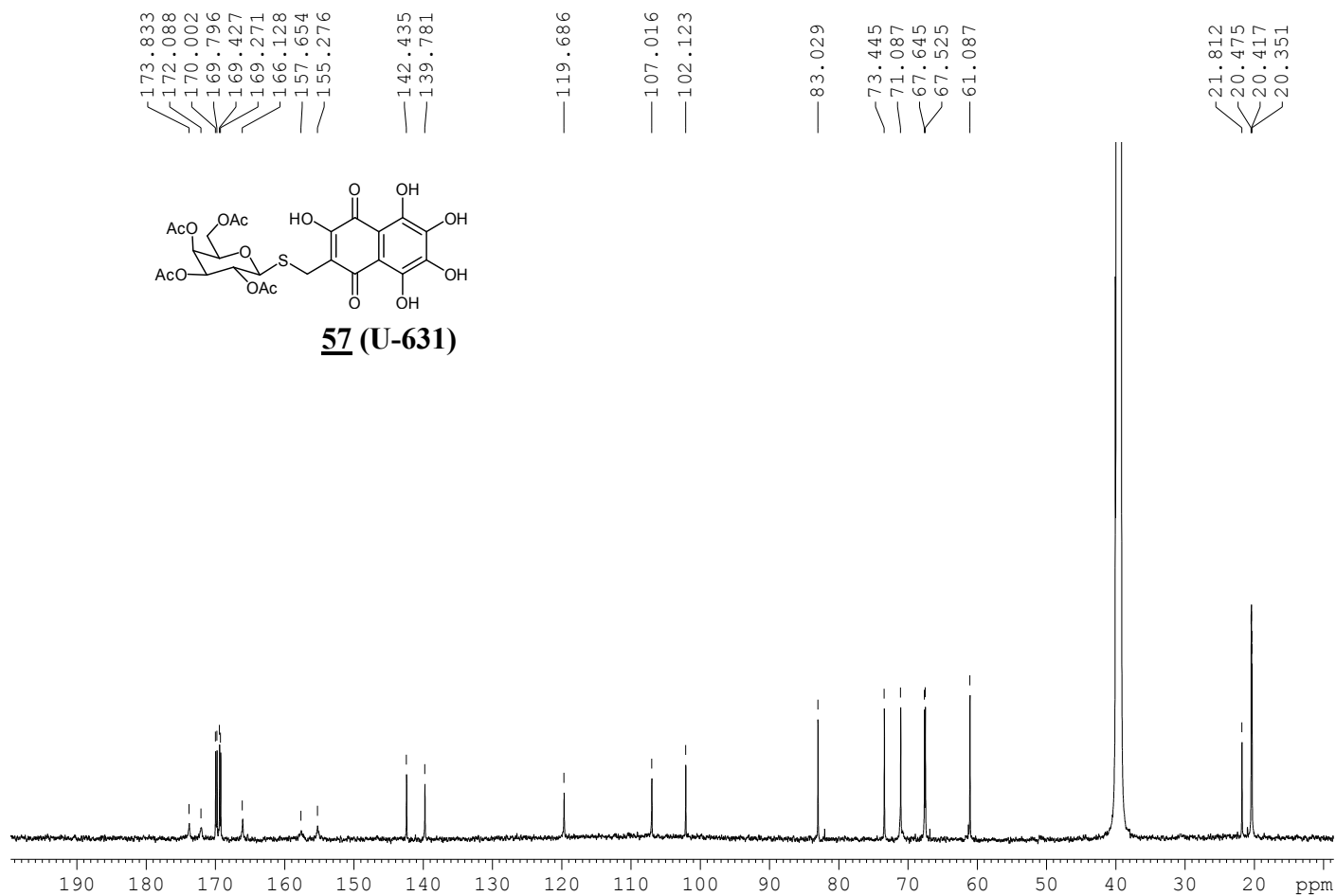
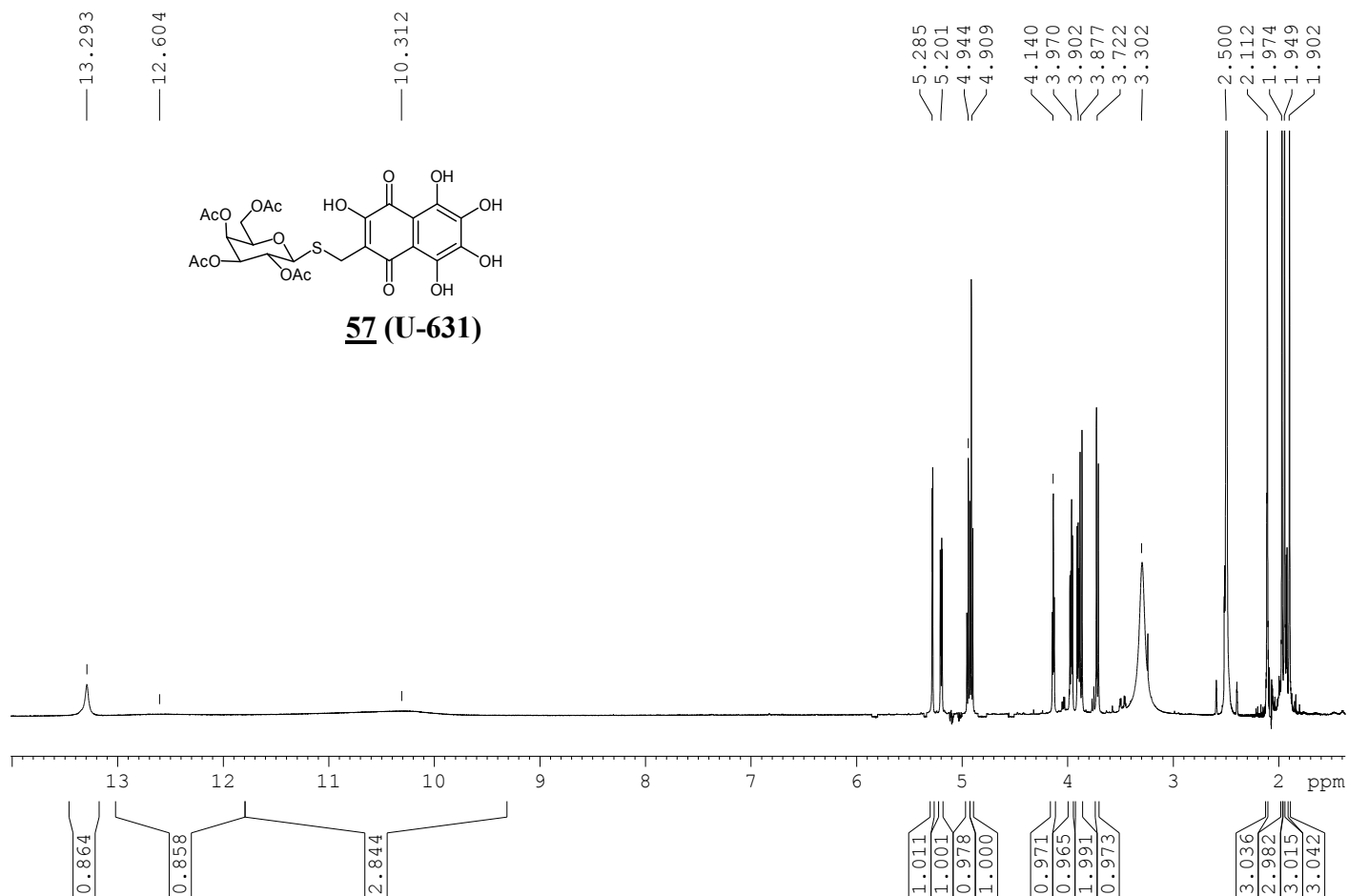
3-(β -D-Glucopyranosyl-1-thiomethyl)-5,8-dihydroxy-2,6,7-trimethoxynaphthalene-1,4-dione **52** (U-641), (^1H NMR - 700 MHz, ^{13}C NMR - 176 MHz, solvent - DMSO- d_6)



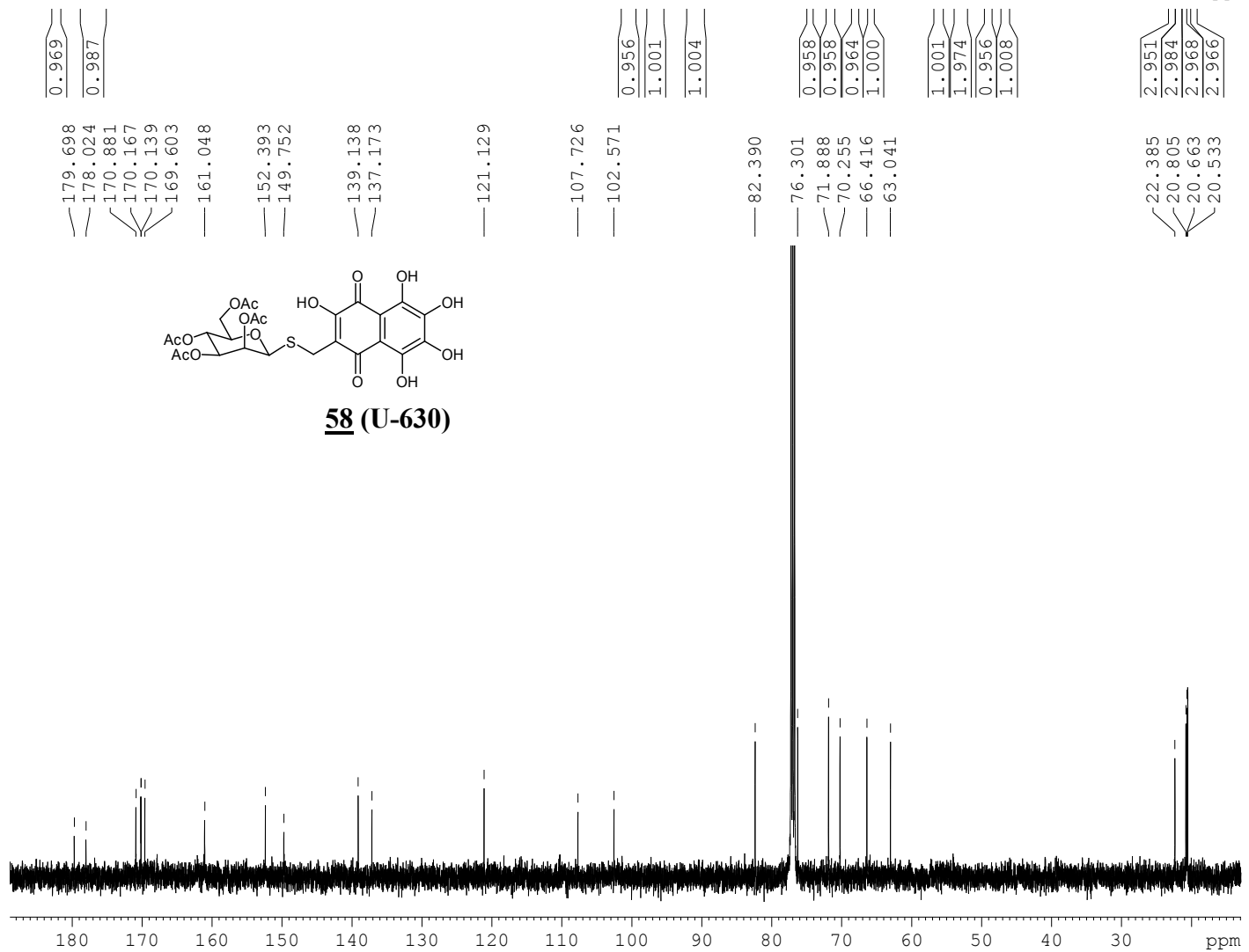
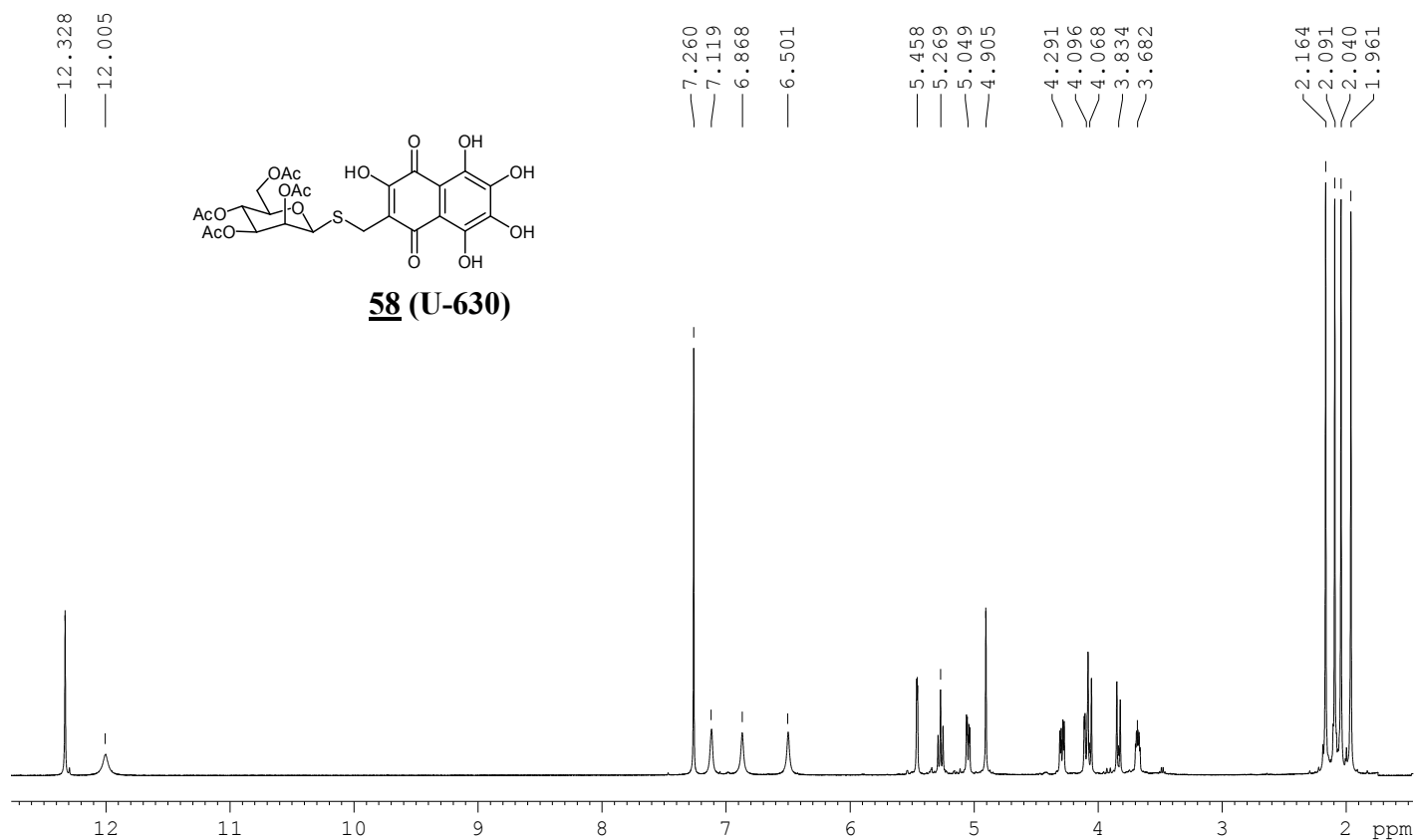
3-(Tetra-O-acetyl- β -D-glucopyranosyl-1-thiomethyl)-2,5,6,7,8-pentahydroxynaphthalene-1,4-dione **56** (U-629), (^1H NMR - 700 MHz, ^{13}C NMR - 176 MHz, solvent - CDCl_3)



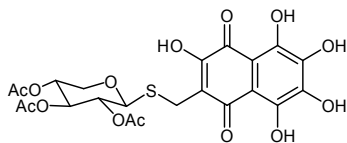
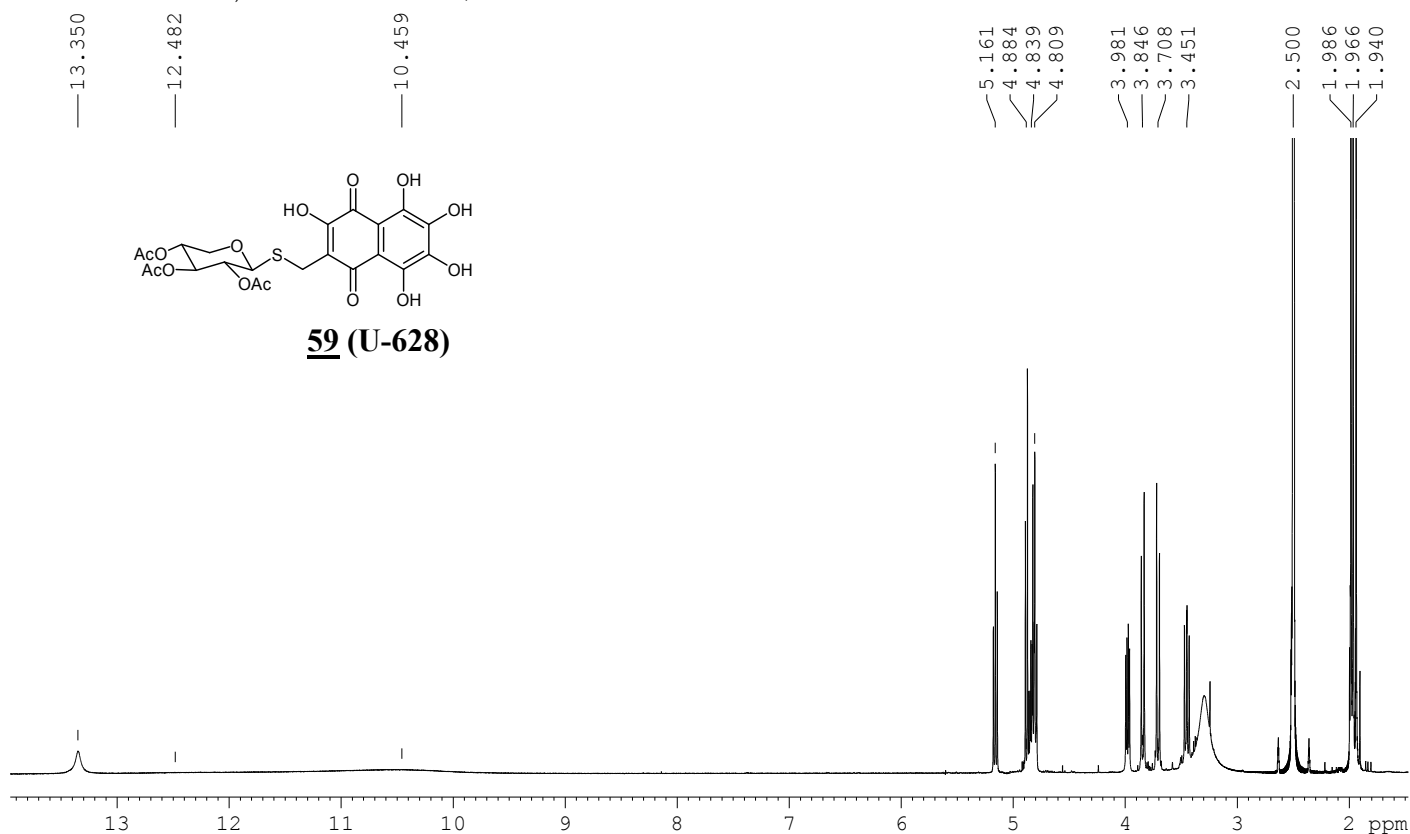
3-(Tetra-O-acetyl- β -D-galactopyranosyl-1-thiomethyl)-2,5,6,7,8-pentahydroxynaphthalene-1,4-dione **57** (U-631), (^1H NMR - 700 MHz, ^{13}C NMR - 176 MHz, solvent - $\text{DMSO-}d_6$)



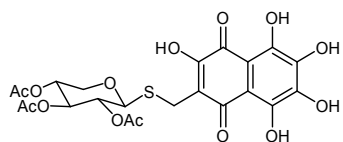
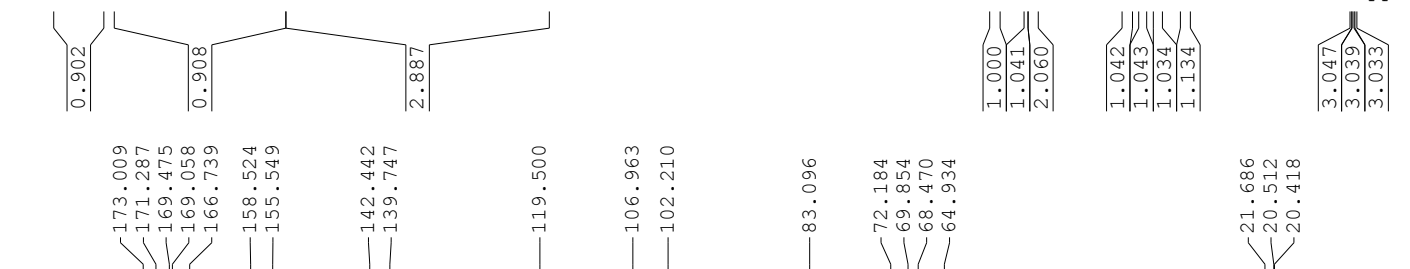
3-(Tetra-O-acetyl- β -D-mannopyranosyl-1-thiomethyl)-2,5,6,7,8-pentahydroxynaphthalene-1,4-dione **58** (U-630), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - CDCl_3)



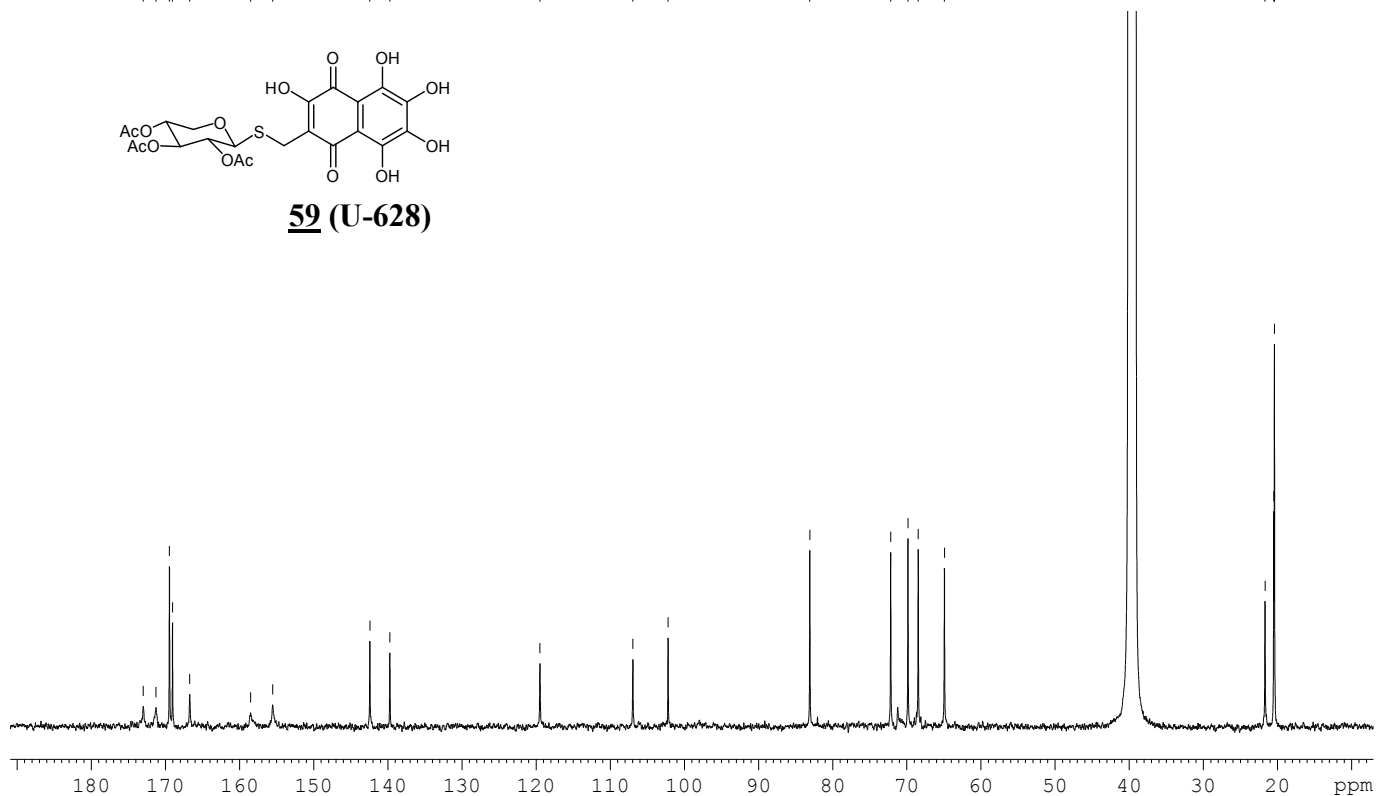
3-(Tri-O-acetyl- β -D-xylopyranosyl-1-thiomethyl)-2,5,6,7,8-pentahydroxynaphthalene-1,4-dione **59** (U-628), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



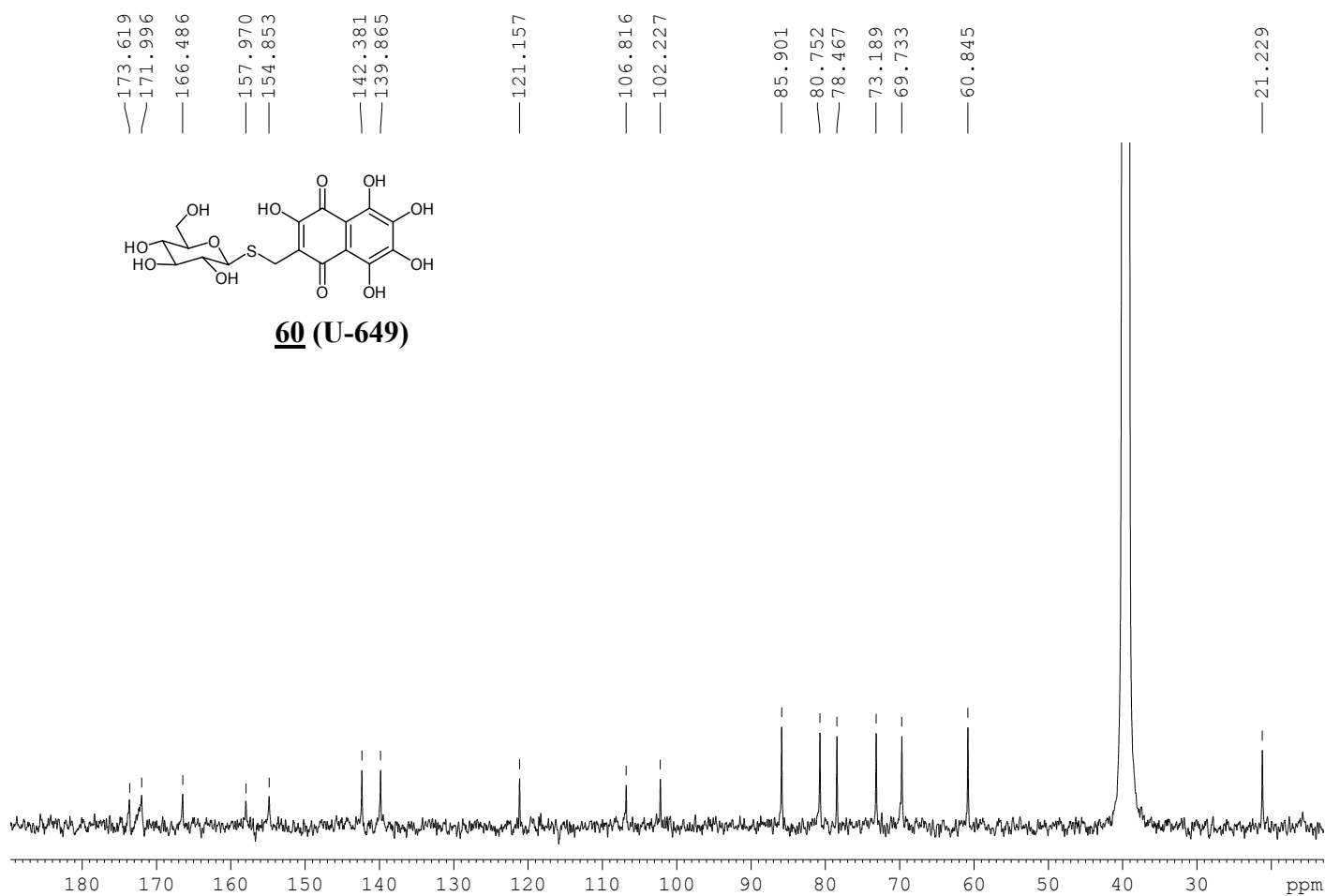
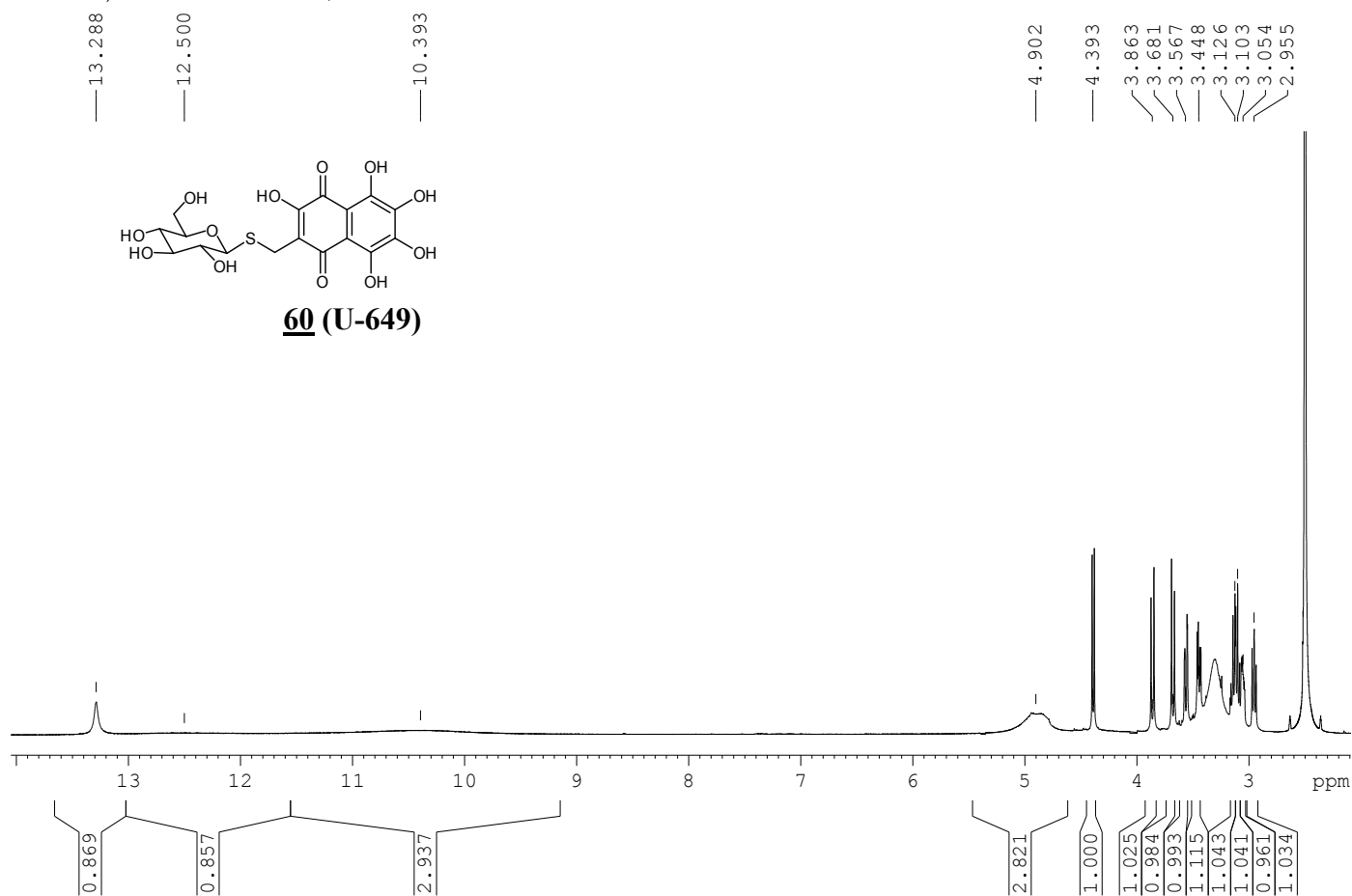
59 (U-628)



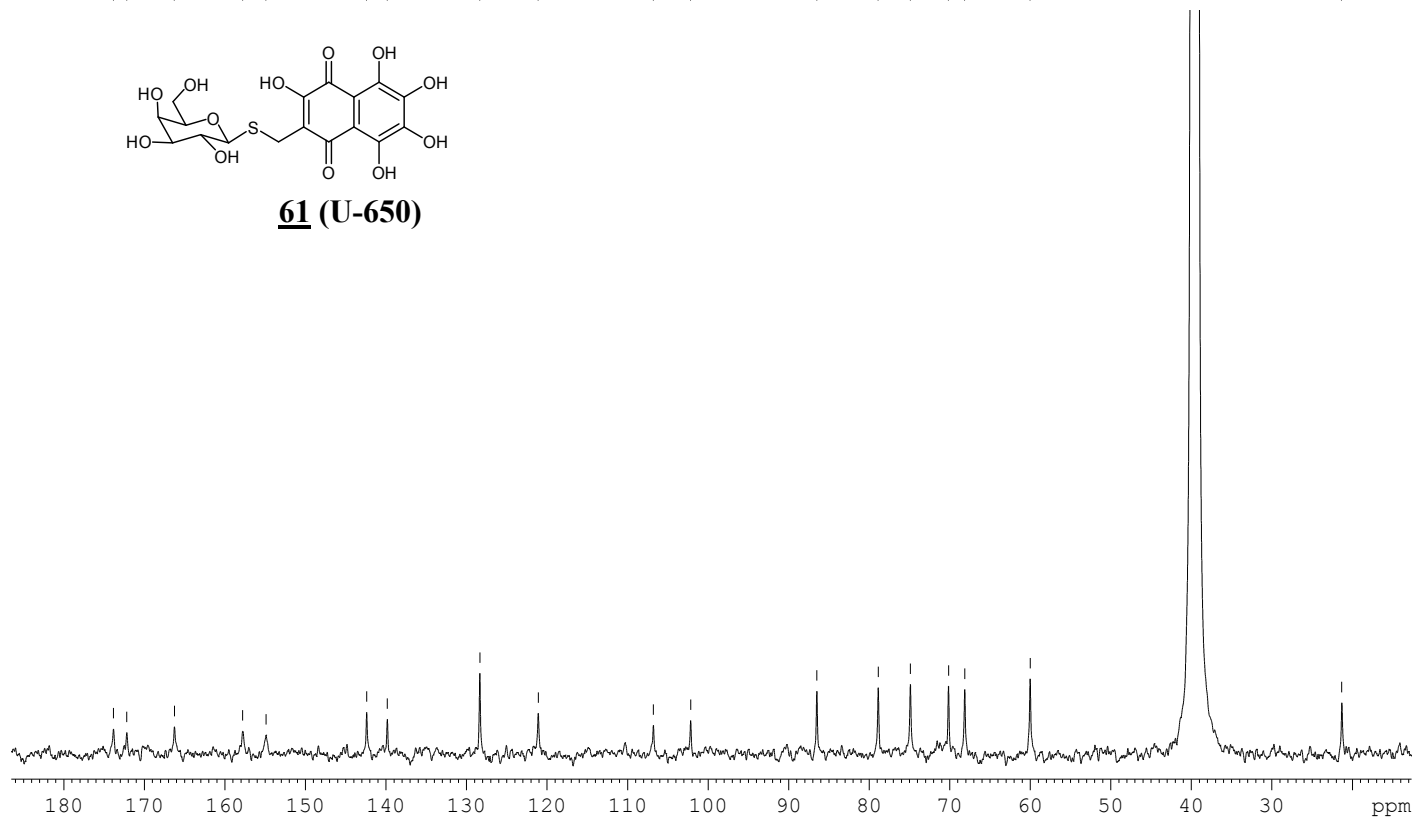
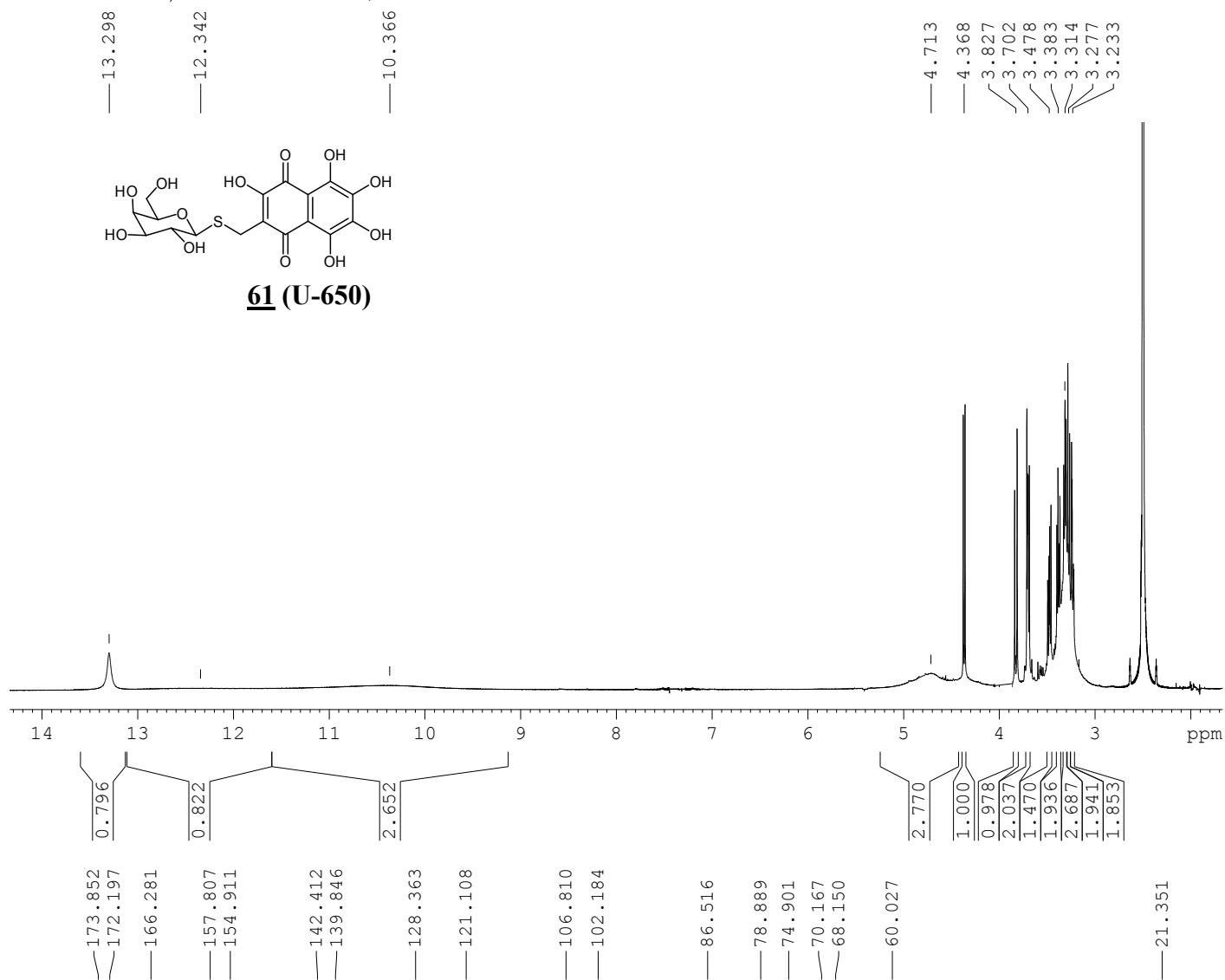
59 (U-628)



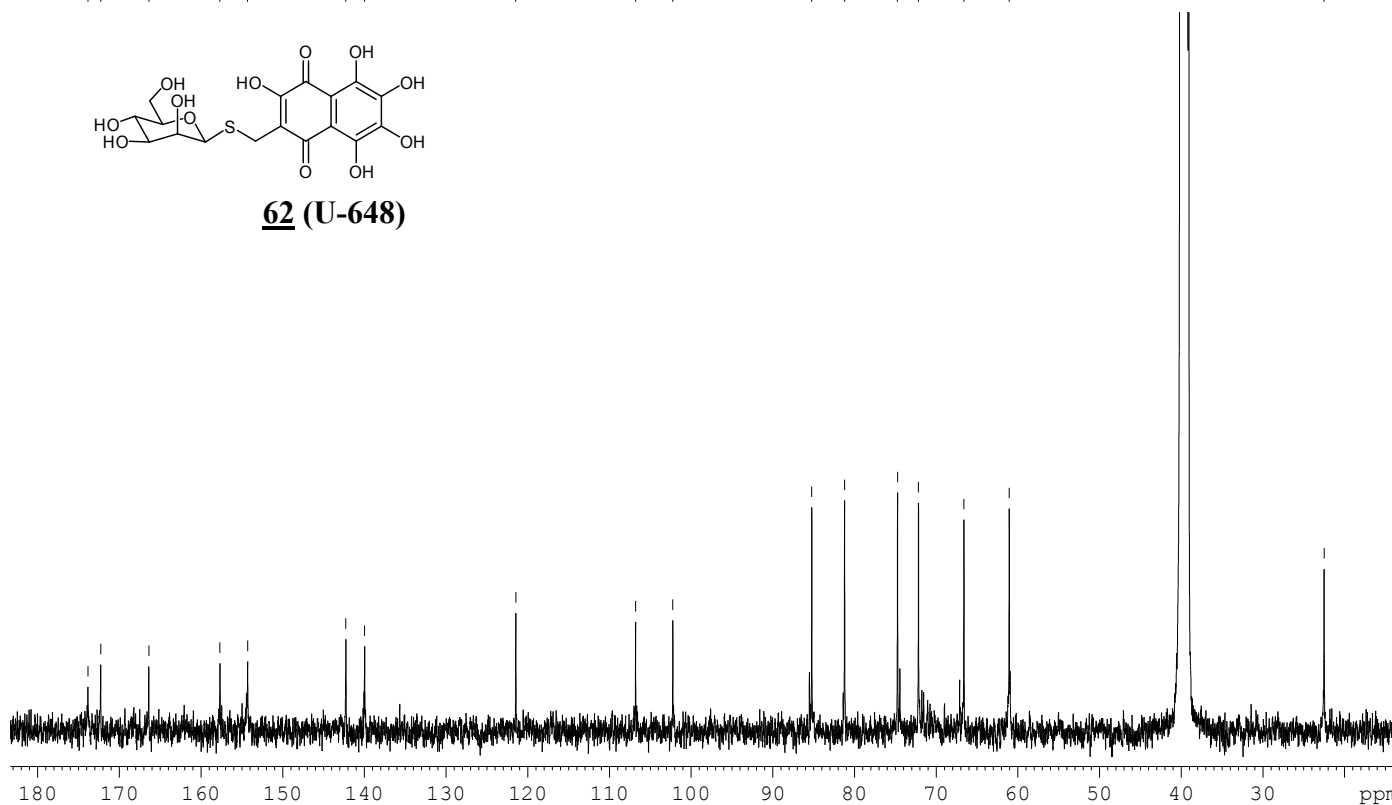
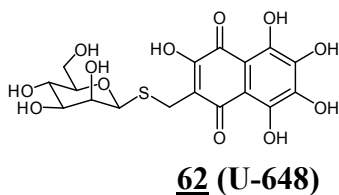
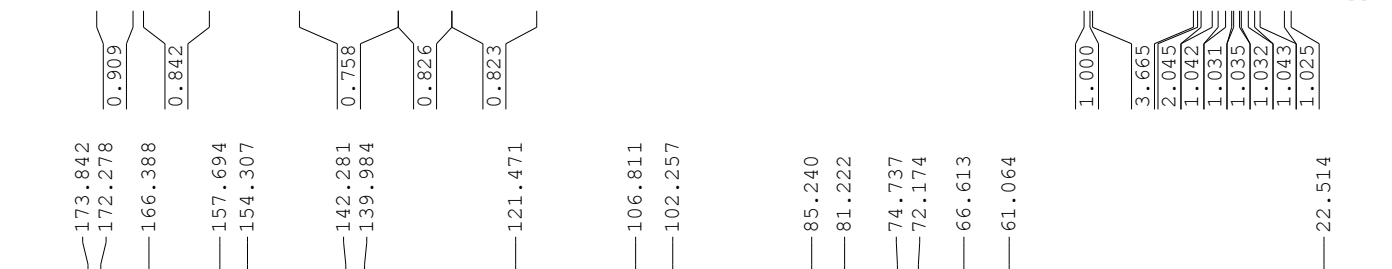
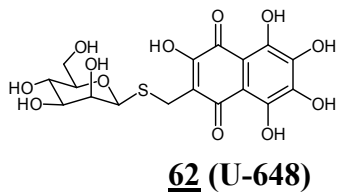
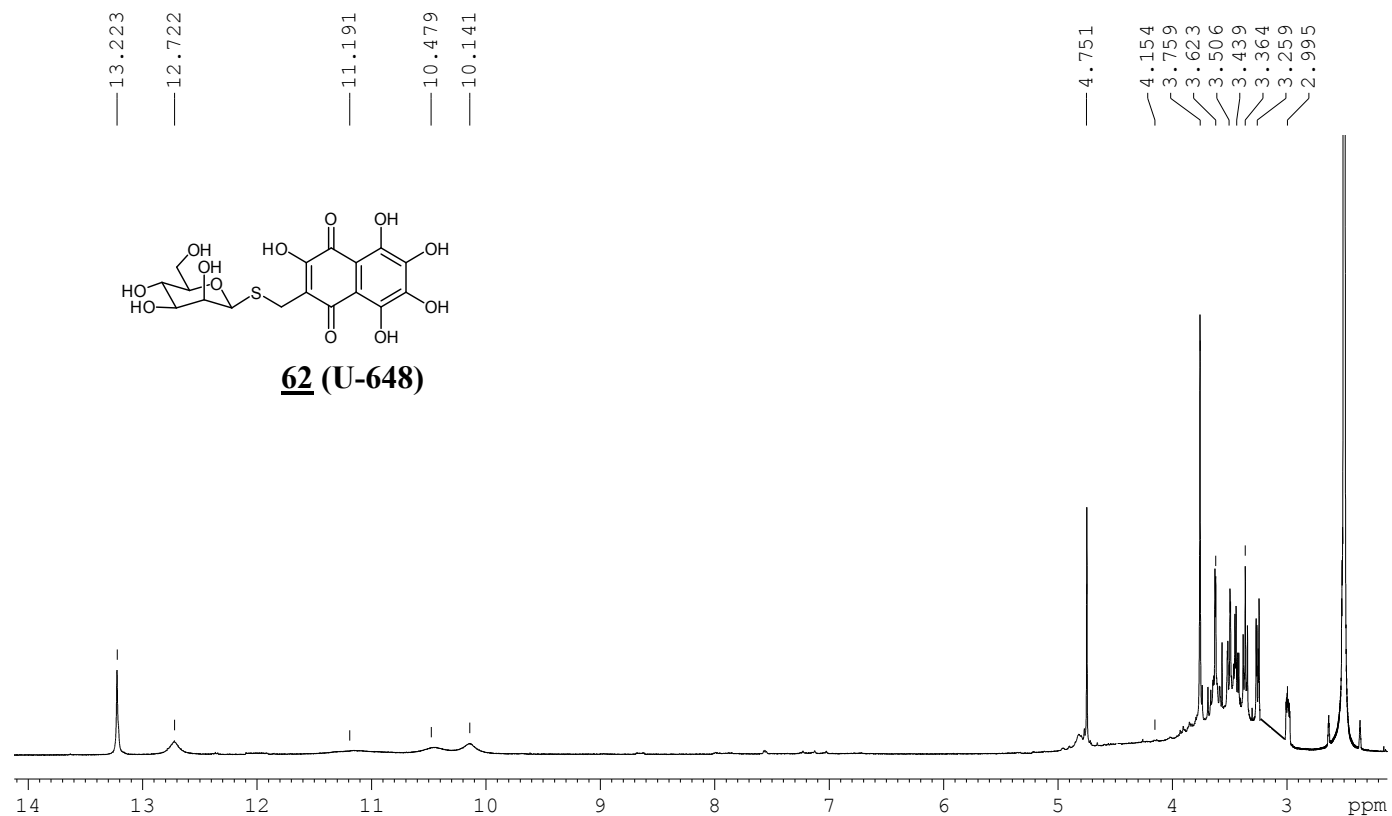
3-(β -D-Glucopyranosyl-1-thiomethyl)-2,5,6,7,8-pentahydroxynaphthalene-1,4-dione **60** (U-649), (^1H NMR - 700 MHz, ^{13}C NMR - 176 MHz, solvent - DMSO- d_6)



3-(β -D-Galactopyranosyl-1-thiomethyl)-2,5,6,7,8-pentahydroxynaphthalene-1,4-dione **61** (U-650), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



3-(β -D-Mannopyranosyl-1-thiomethyl)-2,5,6,7,8-pentahydroxynaphthalene-1,4-dione **62** (U-648), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)



3-(β -D-Xylopyranosyl-1-thiomethyl)-2,5,6,7,8-pentahydroxynaphthalene-1,4-dione **63** (U-647), (^1H NMR - 500 MHz, ^{13}C NMR - 125 MHz, solvent - DMSO- d_6)

